

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

***** Welcome to STN International *****

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS	3	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	5	AUG 24	CA/CAPLUS enhanced with legal status information for U.S. patents
NEWS	6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS	7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS	8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS	9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS	10	NOV 23	Addition of SCAN format to selected STN databases
NEWS	11	NOV 23	Annual Reload of IFI Databases
NEWS	12	DEC 01	FRFULL Content and Search Enhancements
NEWS	13	DEC 01	DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets
NEWS	14	DEC 02	Derwent World Patent Index: Japanese FI-TERM thesaurus added
NEWS	15	DEC 02	PCTGEN enhanced with patent family and legal status display data from INPADOCDB
NEWS	16	DEC 02	USGENE: Enhanced coverage of bibliographic and sequence information
NEWS	17	DEC 21	New Indicator Identifies Multiple Basic Patent Records Containing Equivalent Chemical Indexing in CA/CAPLUS
NEWS	18	JAN 12	Match STN Content and Features to Your Information Needs, Quickly and Conveniently
NEWS	19	JAN 25	Annual Reload of MEDLINE database
NEWS	20	FEB 16	STN Express Maintenance Release, Version 8.4.2, Is Now Available for Download
NEWS	21	FEB 16	Derwent World Patents Index (DWPI) Revises Indexing of Author Abstracts
NEWS	22	FEB 16	New FASTA Display Formats Added to USGENE and PCTGEN
NEWS	23	FEB 16	INPADOCDB and INPAFAMDB Enriched with New Content and Features
NEWS	24	FEB 16	INSPEC Adding Its Own IPC codes and Author's E-mail Addresses
NEWS	25	APR 02	CAS Registry Number Crossover Limits Increased to 500,000 in Key STN Databases
NEWS	26	APR 02	PATDPAFULL: Application and priority number formats enhanced
NEWS	27	APR 02	PATDPAFULL has been enhanced with front page images
NEWS	28	APR 02	DWPI: New display format ALLSTR available
NEWS	29	APR 02	New Thesaurus Added to Derwent Databases for Smooth Sailing through U.S. Patent Codes

NEWS 30 APR 02 EMBASE Adds Unique Records from MEDLINE, Expanding
Coverage back to 1948

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that
specific topic.

All use of STN is subject to the provisions of the STN customer
agreement. This agreement limits use to scientific research. Use
for software development or design, implementation of commercial
gateways, or use of CAS and STN data in the building of commercial
products is prohibited and may result in loss of user privileges
and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 05:07:01 ON 07 APR 2010

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 05:07:13 ON 07 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0
DICTIONARY FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdnoc/properties.html>

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.49	0.71

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 05:07:20 ON 07 APR 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

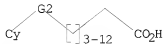
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 05:19:04 ON 07 APR 2010
FILE 'REGISTRY' ENTERED AT 05:19:04 ON 07 APR 2010
COPYRIGHT (C) 2010 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.49	0.71

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 pt VII Amended genus.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,N
G2 O,S,N,[@1-@2]

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 05:19:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 91197 TO ITERATE

2.2% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

35 ANSWERS

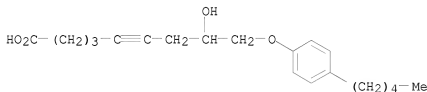
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1805965 TO 1841915
PROJECTED ANSWERS: 29522 TO 34314

L2 35 SEA SSS SAM L1

=> d scan

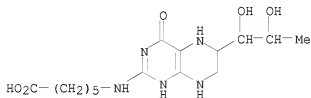
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5-Nonynoic acid, 8-hydroxy-9-(4-pentylphenoxy)-
MF C20 H28 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

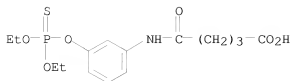
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Hexanoic acid, 6-[[6-(1,2-dihydroxypropyl)-3,4,5,6,7,8-hexahydro-4-oxo-2-
pteridinyl]amino]-
MF C15 H25 N5 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pentanoic acid, 5-[[3-[(diethoxyphosphinothioyl)oxy]phenyl]amino]-5-oxo-
MF C15 H22 N O6 P S

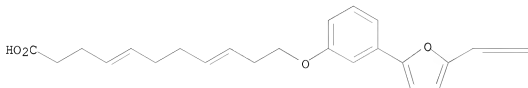


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

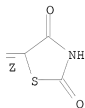
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 4,8-Undecadienoic acid, 11-[3-[5-[(Z)-(2,4-dioxo-5-
 thiazolidinylidene)methyl]-2-furanyl]phenoxy]-
 MF C25 H25 N O6 S

Double bond geometry as described by E or Z.

PAGE 1-A



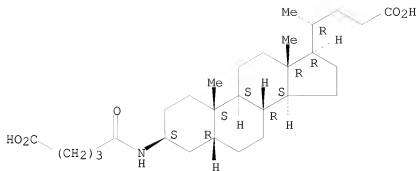
PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

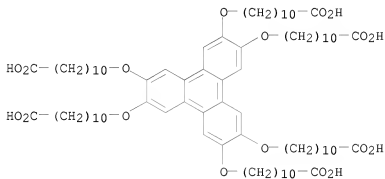
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Cholan-24-oic acid, 3-[(4-carboxy-1-oxobutyl)amino]-, potassium salt
 (1:2), (3β,5β)-
 MF C29 H47 N O5 . 2 K

Absolute stereochemistry.



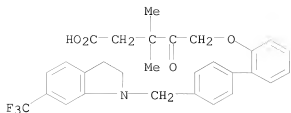
● 2 K

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Undecanoic acid, 11,11',11'',11''',11'''',11''''',11''''''-[2,3,6,7,10,11-
 triphenylenehexaylhexakis(oxy)]hexakis-
 MF C84 H132 O18



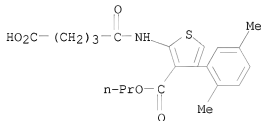
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[[4'-[[[2,3-dihydro-6-(trifluoromethyl)-1H-indol-1-
 yl]methyl][1,1'-biphenyl]-2-yl]oxy]-3,3-dimethyl-4-oxo-
 MF C29 H28 F3 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

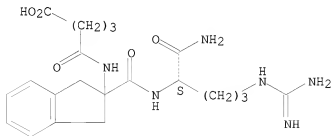
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Thiophenecarboxylic acid, 2-((4-carboxy-1-oxobutyl)amino)-4-(2,5-
dimethylphenyl)-, 3-propyl ester
MF C21 H25 N O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pentanoic acid, 5-[[2-[[[(1S)-1-(aminocarbonyl)-4-
|(aminoininomethyl)amino]butyl]amino]carbonyl]-2,3-dihydro-1H-inden-2-
yl]amino]-5-oxo-
MF C21 H30 N6 O5

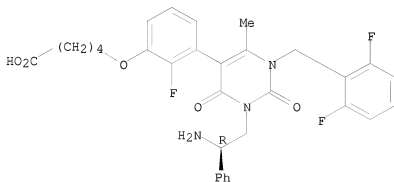
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[3-[3-[(2R)-2-amino-2-phenylethyl]-1-[(2,6-difluorophenyl)methyl]-1,2,3,4-tetrahydro-6-methyl-2,4-dioxo-5-pyrimidinyl]-2-fluorophenoxy]-
 MF C31 H30 F3 N3 O5
 CI COM

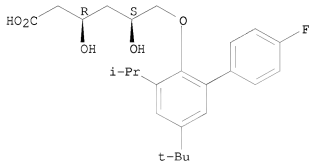
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN D-erythro-Hexonic acid, 2,4-dideoxy-6-O-[5-(1,1-dimethylethyl)-4'-fluoro-3-(1-methylethyl)[1,1'-biphenyl]-2-yl]-
 MF C25 H33 F O5
 CI COM

Absolute stereochemistry.

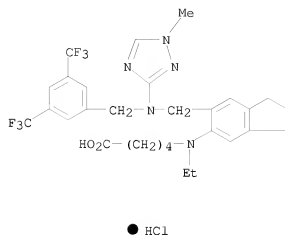


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

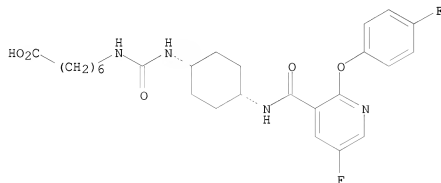
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[6-[[[3,5-bis(trifluoromethyl)phenyl)methyl](1-methyl-1H-1,2,4-triazol-3-yl)amino)methyl]-2,3-dihydro-1H-inden-5-yl]ethylamino]-

, hydrochloride (1:1)
 MF C29 H33 F6 N5 O2 . Cl H



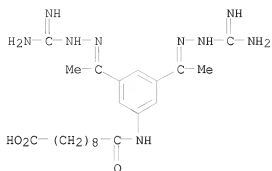
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Heptanoic acid, 7-[[[cis-4-[[[5-fluoro-2-(4-fluorophenoxy)-3-pyridinyl]carbonyl]amino]cyclohexyl]amino]carbonyl]amino]-
 MF C26 H32 F2 N4 O5

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Decanoic acid, 10-[[[3,5-bis[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]phenyl]amino]-10-oxo-,
 hydrochloride (1:2)
 MF C22 H35 N9 O3 . 2 Cl H

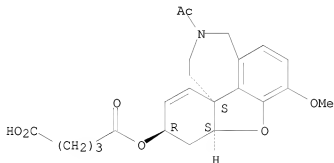


● 2 HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanedioic acid, 1-[(4aS,6R,8aS)-11-acetyl-4a,5,9,10,11,12-hexahydro-3-methoxy-6H-benzofuro[3a,3,2-ef][2]benzazepin-6-yl] ester
 MF C23 H27 N O7

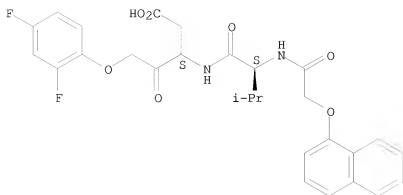
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

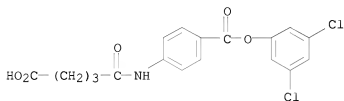
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-(2,4-difluorophenoxy)-3-[[2S]-3-methyl-2-[[2-(1-naphthalenyloxy)acetyl]amino]-1-oxobutyl]amino]-4-oxo-, (3S)-
 MF C28 H28 F2 N2 O7

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

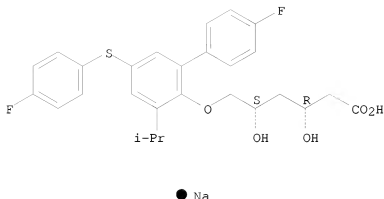
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzoic acid, 4-[(4-carboxy-1-oxobutyl)amino]-, 1-(3,5-dichlorophenyl)
 ester
 MF C18 H15 Cl2 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN D-erythro-Hexonic acid, 2,4-dideoxy-6-O-[(4'-fluoro-5-[(4-
 fluorophenyl)thio]-3-(1-methylethyl)[1,1'-biphenyl]-2-yl]-, monosodium
 salt (9CI)
 MF C27 H28 F2 O5 S . Na

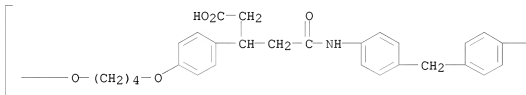
Absolute stereochemistry.



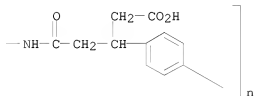
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Poly[oxy-1,4-butanediyl-oxy-1,4-phenylene[1-(carboxymethyl)-3-oxo-1,3-propanediyl]imino-1,4-phenylenemethylene-1,4-phenyleneimino[3-(carboxymethyl)-1-oxo-1,3-propanediyl]-1,4-phenylene] (9CI)
 MF (C39 H40 N2 O8)n
 CI PMS

RELATED POLYMERS AVAILABLE WITH POLYLINK

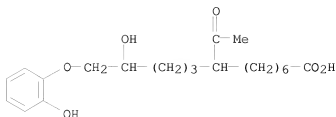
PAGE 1-A



PAGE 1-B

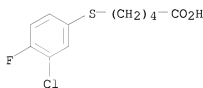


L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Tridecanoic acid, 8-acetyl-12-hydroxy-13-(2-hydroxyphenoxy)-
 MF C21 H32 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

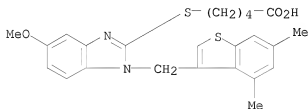
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[(3-chloro-4-fluorophenyl)thio]-
 MF C11 H12 Cl F O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

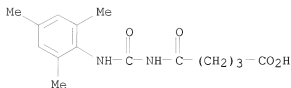
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):15

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[1-[(4,6-dimethylbenzo[b]thien-3-yl)methyl]-5-methoxy-
 1H-benzimidazol-2-yl]thio]-
 MF C24 H26 N2 O3 S2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

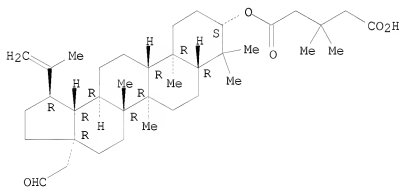
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-oxo-5-[[[(2,4,6-trimethylphenyl)amino]carbonyl]amino]-
 MF C15 H20 N2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Lup-20(29)-ene-28-carboxaldehyde, 3-(4-carboxy-3,3-dimethyl-1-oxobutoxy)-,
 (3β)-
 MF C38 H60 O5

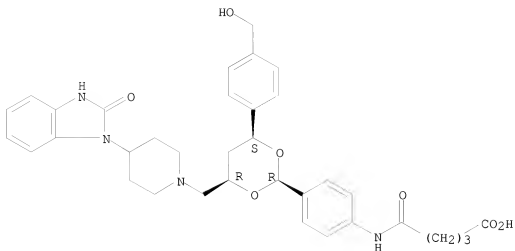
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

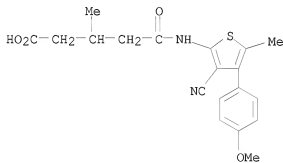
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[4-[(2R,4R,6S)-4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)-1-piperidinyl]methyl]-6-[4-(hydroxymethyl)phenyl]-1,3-dioxan-2-yl]phenyl]amino]-5-oxo-
 MF C35 H40 N4 O7

Absolute stereochemistry.



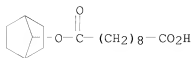
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[3-cyano-4-(4-methoxyphenyl)-5-methyl-2-thienyl]amino]-
 3-methyl-5-oxo-
 MF C19 H20 N2 O4 S



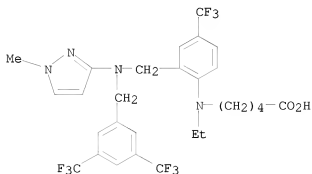
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Decanedioic acid, 1-bicyclo[2.2.1]hept-7-yl ester
 MF C17 H28 O4



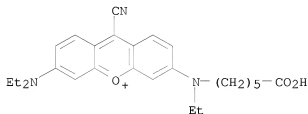
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[2-[[[3,5-bis(trifluoromethyl)phenyl]methyl](1-methyl-
 1H-pyrazol-3-yl)amino]methyl]-4-(trifluoromethyl)phenyl]ethylamino]-
 MF C28 H29 F9 N4 O2
 CI COM

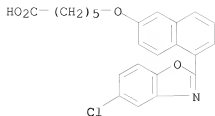


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Xanthylium, 3-[(5-carboxypentyl)ethylamino]-9-cyano-6-(diethylamino)-
 MF C26 H32 N3 O3
 CI COM

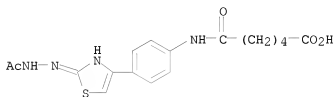


L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Hexanoic acid, 6-[[5-(5-chloro-2-benzoxazolyl)-2-naphthalenyl]oxy]-,
 sodium salt (1:1)
 MF C23 H20 Cl N O4 . Na



● Na

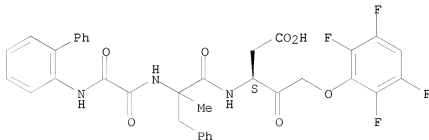
L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Hexanoic acid, 6-[[4-[2-(2-acetylhydrazinyl)-4-thiazolyl]phenyl]amino]-6-oxo-
 MF C17 H20 N4 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 3-[[2-[[2-([1,1'-biphenyl]-2-ylamino)-2-oxoacetyl]amino]-2-methyl-1-oxo-3-phenylpropyl]amino]-4-oxo-5-(2,3,5,6-tetrafluorophenoxy)-, (3S)-
 MF C35 H29 F4 N3 O7

Absolute stereochemistry.

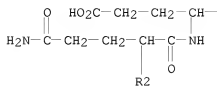
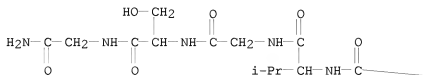


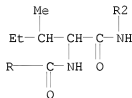
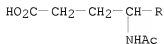
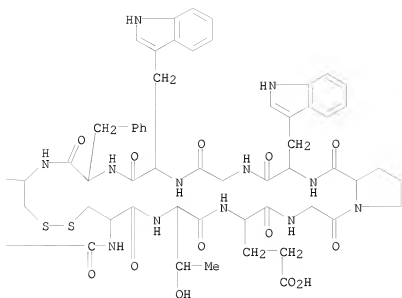
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Glycinamide, N-acetyl-L- α -glutamyl-L-isoleucyl-L-glutamyl-L-
 α -glutamyl-L-cysteinyl-L-threonyl-L- α -glutamylglycyl-L-prolyl-
 L-tryptophylglycyl-L-tryptophyl-L-phenylalanyl-L-cysteinyl-L-valylglycyl-L-
 seryl-, cyclic (5-14)-disulfide (9CI)
 SQL 18
 MF C90 H122 N22 O28 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

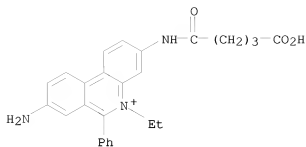
PAGE 1-A



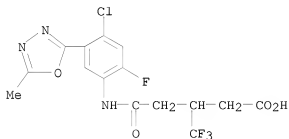


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Phenanthridinium, 8-amino-3-[(4-carboxy-1-oxobutyl)amino]-5-ethyl-6-phenyl-
MF , bromide (1:1)
C26 H26 N3 O3 . Br



L2 35 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Pentanoic acid, 5-[[4-chloro-2-fluoro-5-(5-methyl-1,3,4-oxadiazol-2-yl)phenyl]amino]-5-oxo-3-(trifluoromethyl)-
 MF C15 H12 Cl F4 N3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l1 sss full
 FULL SEARCH INITIATED 05:21:32 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 1822843 TO ITERATE

73.4% PROCESSED	1338751 ITERATIONS	20942 ANSWERS
93.9% PROCESSED	1712226 ITERATIONS	24266 ANSWERS
99.0% PROCESSED	1805079 ITERATIONS	24699 ANSWERS
100.0% PROCESSED	1822843 ITERATIONS	24701 ANSWERS

SEARCH TIME: 00.01.08

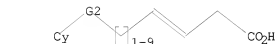
L3 24701 SEA SSS FUL L1

=> save temp 13 masterset/a
ANSWER SET L3 HAS BEEN SAVED AS 'MASTERSSET/A'

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 pt VII bg unsat.str

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



G1 O,N
G2 O,S,N,[@1-@2]

Structure attributes must be viewed using STN Express query preparation.

=> search l4 sss sam subset = l3
SAMPLE SUBSET SEARCH INITIATED 05:28:53 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 19 TO ITERATE

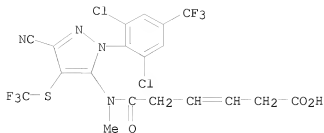
100.0% PROCESSED 19 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):	ONLINE	**COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):	119 TO	641
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):	22 TO	418

L5 11 SEA SUB=L3 SSS SAM L4

=> d scan

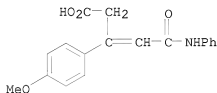
L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 6-[[3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-
[(trifluoromethyl)thio]-1H-pyrazol-5-yl]methylamino]-6-oxo-
MF C19 H12 C12 F6 N4 O3 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

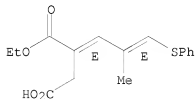
L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy-β-[2-oxo-2-(phenylamino)ethylidene]-
 MF C18 H17 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Butanedioic acid, 2-[(2E)-2-methyl-3-(phenylthio)-2-propen-1-ylidene]-,
 1-ethyl ester, (2E)-
 MF C16 H18 O4 S

Double bond geometry as shown.

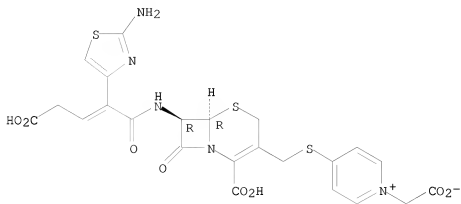


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

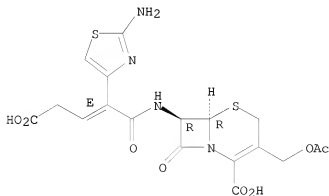
IN Pyridinium, 4-[[[7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]thio]-1-(carboxymethyl)-, inner salt, (6R-trans)- (9CI)
MF C23 H21 N5 O8 S3

Absolute stereochemistry.
Double bond geometry unknown.



L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(acetyloxy)methyl]-7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-, [6R-[6α,7β(E)]]-, (9CI)
MF C18 H18 N4 O8 S2

Absolute stereochemistry.
Double bond geometry as shown.

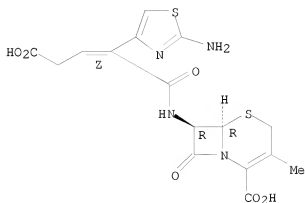


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-3-methyl-8-

oxo-, [6R-[6 α ,7 β (Z)]]- (9CI)
 MF C16 H16 N4 O6 S2

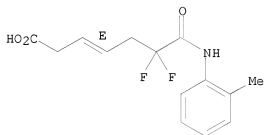
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Heptenoic acid, 6,6-difluoro-7-[(2-methylphenyl)amino]-7-oxo-, (3E)-
 MF C14 H15 F2 N O3

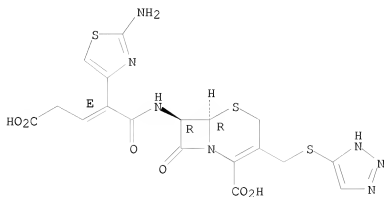
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[[(2E)-2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-buten-1-yl]amino]-8-oxo-
 3-[(1H-1,2,3-triazol-5-ylthio)methyl]-, (6R,7R)-
 MF C18 H17 N7 O6 S3
 CI COM

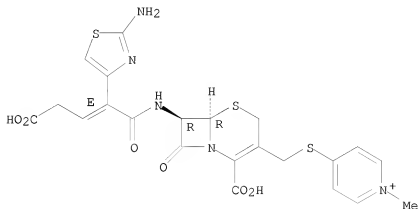
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[[[7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]thio]-1-methyl-, [6R-[6 α ,7 β (E)]]- (9CI)
MF C22 H22 N5 O6 S3

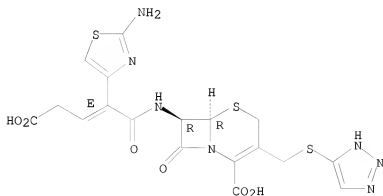
Absolute stereochemistry.
Double bond geometry as shown.



L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-3-[[1H-1,2,3-triazol-4-ylthio)methyl]-, disodium salt, [6R-[6 α ,7 β (E)]]- (9CI)

MF C18 H17 N7 O6 S3 . 2 Na

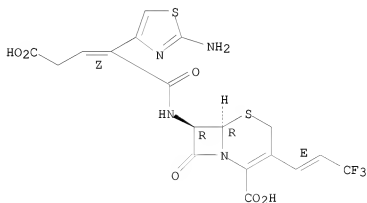
Absolute stereochemistry.
Double bond geometry as shown.



● 2 Na

L5 11 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-3-
(3,3,3-trifluoro-1-propenyl)-, [6R-[3(E),6 α ,7 β (Z)]]- (9CI)
MF C18 H15 F3 N4 O6 S2

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search 14 sss full subset = 13
FULL SUBSET SEARCH INITIATED 05:31:21 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 438 TO ITERATE

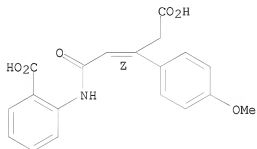
100.0% PROCESSED 438 ITERATIONS 222 ANSWERS
SEARCH TIME: 00.00.01

L6 222 SEA SUB=L3 SSS FUL L4

=> d scan

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepropanoic acid, β -[2-[(2-carboxyphenyl)amino]-2-oxoethylidene]-
4-methoxy-, (β Z)-
MF C19 H17 N O6

Double bond geometry as shown.

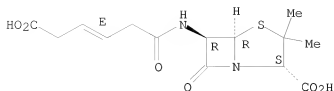


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid,
6-[[[(3E)-5-carboxy-1-oxo-3-penten-1-yl]amino]-3,3-dimethyl-7-oxo-, sodium
salt (1:2), (2S,5R,6R)-
MF C14 H18 N2 O6 S . 2 Na

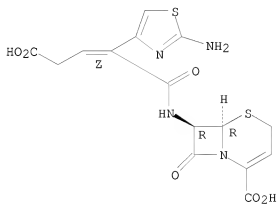
Absolute stereochemistry.
Double bond geometry as shown.



●2 Na

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-,
 sodium salt, [6R-[6 α ,7 β (Z)]]- (9CI)
 MF C15 H14 N4 O6 S2 . x Na

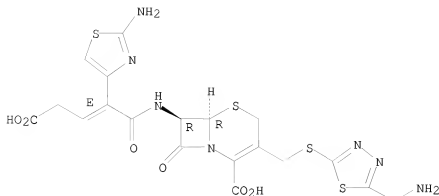
Absolute stereochemistry.
 Double bond geometry as shown.



●x Na

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[[5-(aminomethyl)-1,3,4-thiadiazol-2-yl]thio]methyl]-7-[[2-(2-amino-4-
 thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-,
 [6R-[6 α ,7 β (E)]]- (9CI)
 MF C19 H19 N7 O6 S4

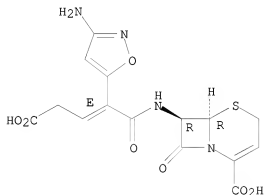
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(3-amino-5-isoxazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-,
 [6R-[6α,7β(E)]]-, (9CI)
 MF C15 H14 N4 O7 S

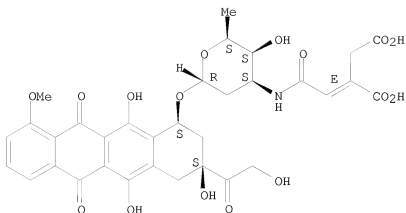
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5,12-Naphthacenedione, 10-[[3-[[2E)-3,4-dicarboxy-1-oxo-2-buten-1-yl]amino]-2,3,6-trideoxy-α-L-lyxo-hexopyranosyl]oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(2-hydroxyacetyl)-1-methoxy-, (8S,10S)-
 MF C33 H33 N O16

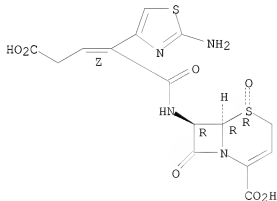
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[[(2Z)-2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-buten-1-yl]amino]-8-oxo-
 , 5-oxide, (5R,6R,7R)-
 MF C15 H14 N4 O7 S2
 CI COM

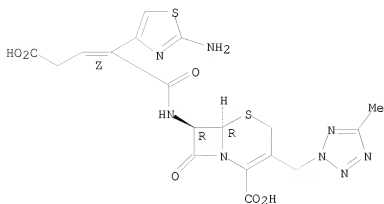
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-3-[(5-methyl-
 2H-tetrazol-2-yl)methyl]-8-oxo-, [6R-[6 α , 7 β (Z)]]- (9CI)
 MF C18 H18 N8 O6 S2

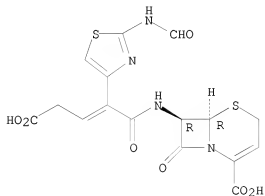
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[4-carboxy-2-[2-(formylamino)-4-thiazolyl]-1-oxo-2-butenyl]amino]-8-oxo-
 , (6R-trans)- (9CI)
 MF C16 H14 N4 O7 S2

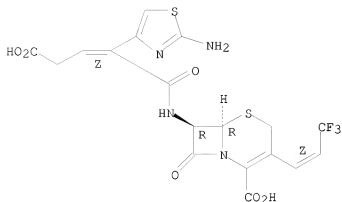
Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

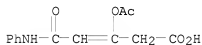
L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-3-
 (3,3,3-trifluoro-1-propenyl)-, [6R-[3(Z),6a,7β(Z)]]- (9CI)
 MF C18 H15 F3 N4 O6 S2

Absolute stereochemistry.
 Double bond geometry as shown.



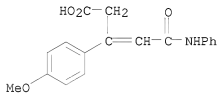
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Penten-3-ol, 3-(acetyloxy)-5-oxo-5-(phenylamino)-
 MF C13 H13 N O5



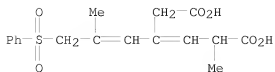
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy-β-[2-oxo-2-(phenylamino)ethylidene]-
 MF C18 H17 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

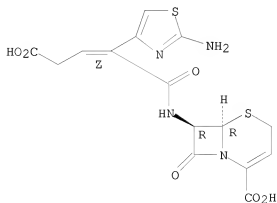
L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenedioic acid, 2-methyl-4-[2-methyl-3-(phenylsulfonyl)-1-propen-1-yl]-
 MF C17 H20 O6 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-,
 trihydrate, [6R-[6 α ,7 β (Z)]]- (9CI)
 MF C15 H14 N4 O6 S2 . 3 H2 O

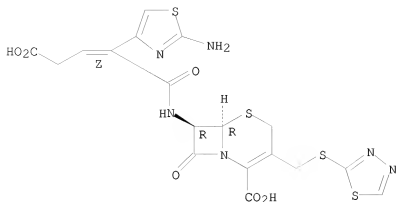
Absolute stereochemistry.
 Double bond geometry as shown.



● 3 H₂O

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-3-
 [(1,3,4-thiadiazol-2-ylthio)methyl]-, [6R-[6 α ,7 β (Z)]]- (9CI)
 MF C18 H16 N6 O6 S4

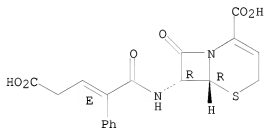
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[(4-carboxy-1-oxo-2-phenyl-2-butenyl)amino]-8-oxo-, disodium salt,
 [6R-[6 α ,7 β (E)]]- (9CI)
 MF C18 H16 N2 O6 S . 2 Na

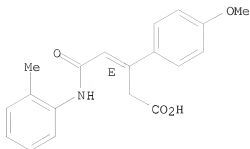
Absolute stereochemistry.
 Double bond geometry as shown.



● 2 Na

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C19 H19 N O4

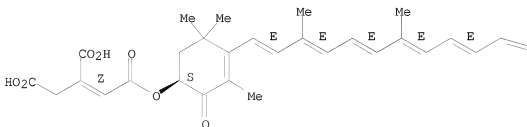
Double bond geometry as shown.



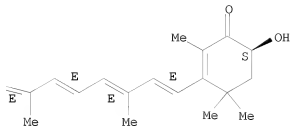
L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN β,β -Carotene-4,4'-dione,
 3-[[(2Z)-3,4-dicarboxy-1-oxo-2-butenyl]oxy]-3'-hydroxy-, (3S,3'S)- (9CI)
 MF C46 H56 O9

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

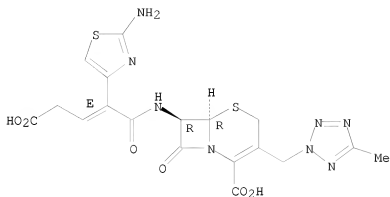


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-3-[(5-methyl-
 2H-tetrazol-2-yl)methyl]-8-oxo-, [6R-[6 α ,7 β (E)]]- (9CI)

MF C18 H18 N8 O6 S2

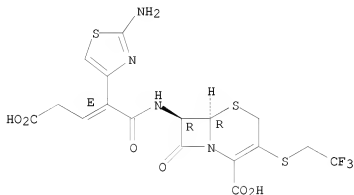
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-butenyl]amino]-8-oxo-3-
[(2,2,2-trifluoroethyl)thio]-, disodium salt, [6R-[6 α ,7 β (E)]]-
(9CI)
MF C17 H15 F3 N4 O6 S3 . 2 Na

Absolute stereochemistry.
Double bond geometry as shown.

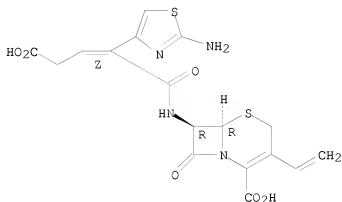


● 2 Na

L6 222 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[(2Z)-2-(2-amino-4-thiazolyl)-4-carboxy-1-oxo-2-buten-1-yl]amino]-3-
 MF ethenyl-8-oxo-, (6R,7R)-
 C17 H16 N4 O6 S2

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

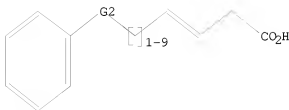
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp l6 mstrunsats/a
 ANSWER SET L6 HAS BEEN SAVED AS 'MSTRUNSATS/A'

=>
 Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
 files\10025947\10025947 pt VII phenyl unsats.str

L7 STRUCTURE UPLOADED

=> d l7
 L7 HAS NO ANSWERS
 L7 STR



G1 O,N

G2 O,S,N,[@1-@2]

Structure attributes must be viewed using STN Express query preparation.

=> search l7 sss sam subset =l6

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> search l7 sss sam subset =l6

SAMPLE SUBSET SEARCH INITIATED 05:37:58 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):

ONLINE **COMPLETE**

PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):

22 TO 418

PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):

3 TO 163

L8 3 SEA SUB=L6 SSS SAM L7

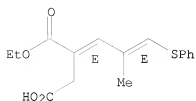
=> d scan

L8 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Butanedioic acid, 2-[(2E)-2-methyl-3-(phenylthio)-2-propen-1-ylidene]-, 1-ethyl ester, (2E)-

MF C16 H18 O4 S

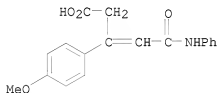
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

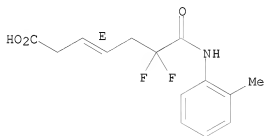
L8 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepropanoic acid, 4-methoxy-β-[2-oxo-2-(phenylamino)ethylidene]-
MF C18 H17 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Heptenoic acid, 6,6-difluoro-7-[(2-methylphenyl)amino]-7-oxo-, (3E)-
MF C14 H15 F2 N O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search 17 sss full subset =16
FULL SUBSET SEARCH INITIATED 05:39:30 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 222 TO ITERATE

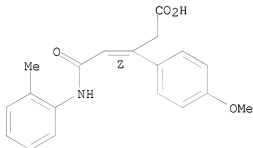
100.0% PROCESSED 222 ITERATIONS 46 ANSWERS
SEARCH TIME: 00.00.01

L9 46 SEA SUB=L6 SSS FUL L7

=> d scan

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepropanoic acid, 4-methoxy- β -[2-[(2-methylphenyl)amino]-2-oxoethylidene]-, (β Z)-
MF C19 H19 N O4

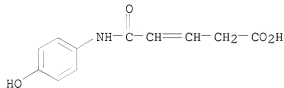
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):46

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Pentenoic acid, 5-[(4-hydroxyphenyl)amino]-5-oxo-
MF C11 H11 N O4

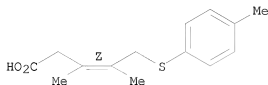


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 3-Pentenoic acid, 3,4-dimethyl-5-[(4-methylphenyl)thio]-, (3Z)-
 MF C14 H18 O2 S

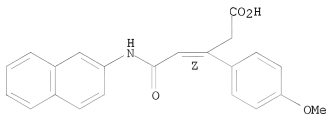
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

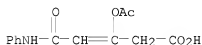
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy-β-[2-(2-naphthalenylamino)-2-oxoethylidene]-, (βZ)-
 MF C22 H19 N O4

Double bond geometry as shown.



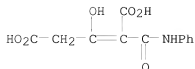
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 3-(acetyloxy)-5-oxo-5-(phenylamino)-
 MF C13 H13 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

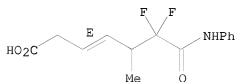
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2-Pentenedioic acid, 3-hydroxy-2-[(phenylamino)carbonyl]-
 MF C12 H11 N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

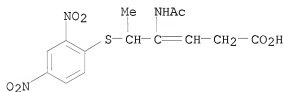
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Heptenoic acid, 6,6-difluoro-5-methyl-7-oxo-7-(phenylamino)-, (3E)-
 MF C14 H15 F2 N O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

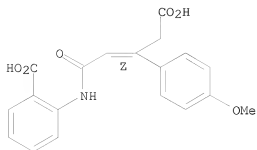
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 4-(acetylamino)-5-[(2,4-dinitrophenyl)thio]-, sodium salt
 (1:1)
 MF C14 H15 N3 O7 S . Na



● Na

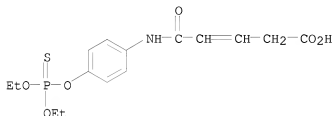
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, β-[2-[(2-carboxyphenyl)amino]-2-oxoethylidene]-
 4-methoxy-, (βZ)-
 MF C19 H17 N O6

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

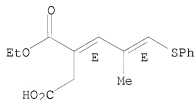
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[4-[(diethoxyphosphinothioyl)oxy]phenyl]amino]-5-oxo-
 MF C15 H20 N O6 P S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Butanedioic acid, 2-[(2E)-2-methyl-3-(phenylthio)-2-propen-1-ylidene]-,
 1-ethyl ester, (2E)-
 MF C16 H18 O4 S

Double bond geometry as shown.

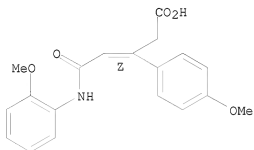


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy-β-[2-[(2-methoxyphenyl)amino]-2-

oxoethylidenel-, (β Z)-
MF C19 H19 N O5

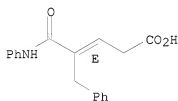
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

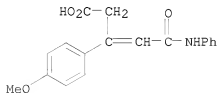
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C18 H17 N O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

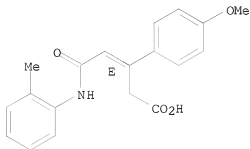
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepropanoic acid, 4-methoxy- β -[2-oxo-2-(phenylamino)ethylidenel]-
MF C18 H17 N O4



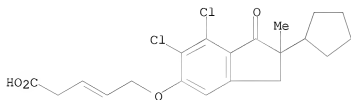
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C19 H19 N O4

Double bond geometry as shown.



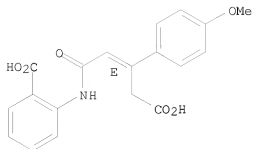
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Pentenoic acid, 5-[(6,7-dichloro-2-cyclopentyl-2,3-dihydro-2-methyl-1-oxo-1H-inden-5-yl)oxy]-
MF C20 H22 Cl2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C19 H17 N O6

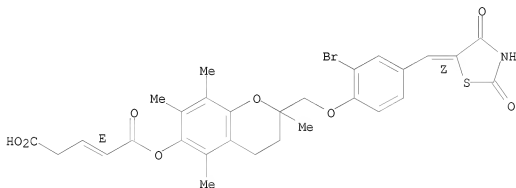
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

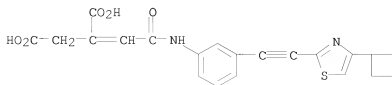
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2-Pentenedioic acid, 1-[2-[[2-bromo-4-[(Z)-(2,4-dioxo-5-
 thiazolidinylidene)methyl]phenoxy]methyl]-3,4-dihydro-2,5,7,8-tetramethyl-
 2H-1-benzopyran-6-yl] ester, (2E)-
 MF C29 H28 Br N O8 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

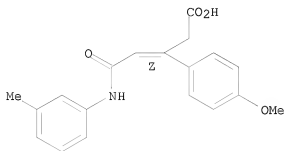
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Butanedioic acid, 2-[2-[[3-[2-(4-cyclobutyl-2-
 thiazolyl)ethynyl]phenyl]amino]-2-oxoethylidene]-
 MF C21 H18 N2 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

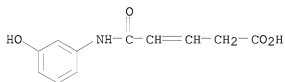
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepropanoic acid, 4-methoxy- β -[2-[(3-methylphenyl)amino]-2-oxoethylidene]-, (β Z)-
MF C19 H19 N O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

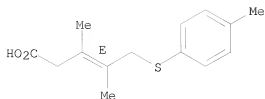
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Pentenoic acid, 5-[(3-hydroxyphenyl)amino]-5-oxo-
MF C11 H11 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Pentenoic acid, 3,4-dimethyl-5-[(4-methylphenyl)thio]-, (3E)-
MF C14 H18 O2 S

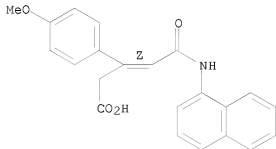
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy- β -[2-(1-naphthalenylamino)-2-oxoethylidene]-, (β Z)-
 MF C22 H19 N O4

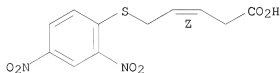
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

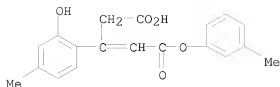
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[(2,4-dinitrophenyl)thio]-, (Z)- (9CI)
 MF C11 H10 N2 O6 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

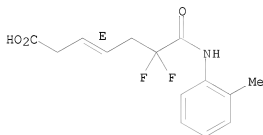
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2-Pentenedioic acid, 3-(2-hydroxy-4-methylphenyl)-, 1-(3-methylphenyl) ester
 MF C19 H18 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

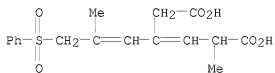
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Heptenoic acid, 6,6-difluoro-7-[(2-methylphenyl)amino]-7-oxo-, (3E)-
 MF C14 H15 F2 N O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

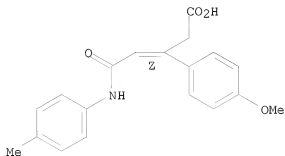
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenedioic acid, 2-methyl-4-[2-methyl-3-(phenylsulfonyl)-1-propen-1-yl]-
 MF C17 H20 O6 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

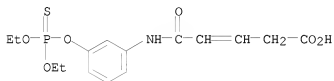
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy-β-[2-[(4-methylphenyl)amino]-2-oxoethylidene]-, (βZ)-
 MF C19 H19 N O4

Double bond geometry as shown.



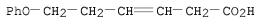
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[[3-[(diethoxyphosphinothioyl)oxy]phenyl]amino]-5-oxo-
 MF C15 H20 N O6 P S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

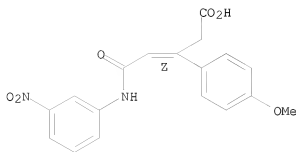
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenoxy-
 MF C12 H14 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

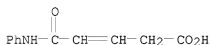
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, 4-methoxy-β-[2-[(3-nitrophenyl)amino]-2-
 oxoethylidene]-, (βZ)-
 MF C18 H16 N2 O6

Double bond geometry as shown.



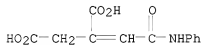
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-oxo-5-(phenylamino)-
 MF C11 H11 N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

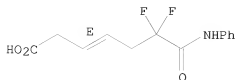
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Butanedioic acid, 2-[2-oxo-2-(phenylamino)ethylidene]-
 MF C12 H11 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

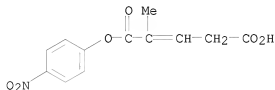
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Heptenoic acid, 6,6-difluoro-7-oxo-7-(phenylamino)-, (3E)-
 MF C13 H13 F2 N O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

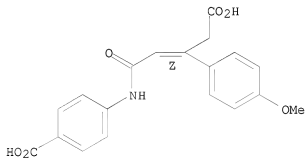
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2-Pentenedioic acid, 2-methyl-, 1-(4-nitrophenyl) ester
 MF C12 H11 N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepropanoic acid, β -[2-[(4-carboxyphenyl)amino]-2-oxoethylidene]-
 4-methoxy-, (βZ)-
 MF C19 H17 N O6

Double bond geometry as shown.

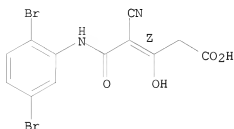


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 4-cyano-5-[(2,5-dibromophenyl)amino]-3-hydroxy-5-oxo-,
 (3Z)-

MF C12 H8 Br2 N2 O4

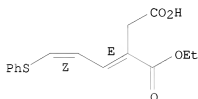
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Butanedioic acid, 2-[(2Z)-3-(phenylthio)-2-propen-1-ylidene]-, 1-ethyl
ester, (2E)-
MF C15 H16 O4 S

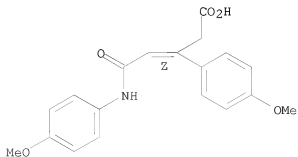
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepropanoic acid, 4-methoxy-β-[2-[(4-methoxyphenyl)amino]-2-oxoethylidene]-, (βZ)-
MF C19 H19 N O5

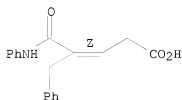
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

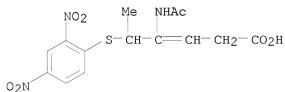
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C18 H17 N O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

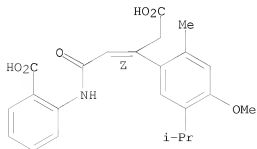
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 4-(acetylamino)-5-[(2,4-dinitrophenyl)thio]-
MF C14 H15 N3 O7 S
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C23 H25 N O6

Double bond geometry as shown.



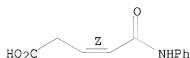
L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-(phenylthio)-
 MF C11 H12 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-oxo-5-(phenylamino)-, (3Z)-
 MF C11 H11 N O3

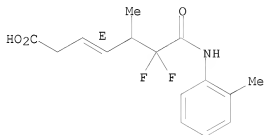
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Heptenoic acid, 6,6-difluoro-5-methyl-7-[(2-methylphenyl)amino]-7-oxo-, (3E)-
 MF C15 H17 F2 N O3

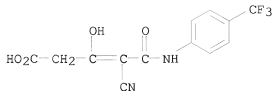
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 46 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 4-cyano-3-hydroxy-5-oxo-5-[[4-(trifluoromethyl)phenyl]amino]-

MF C13 H9 F3 N2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

```
=> e 3-Pentenoic acid, 5-(phenylthio)-/cn
E1      1      3-PENTENOIC ACID, 5-(PHENYLAMINO)-, ETHYL ESTER, (Z)-/CN
E2      1      3-PENTENOIC ACID, 5-(PHENYLMETHOXY)-2-((TRIMETHYLSILYL)METHY
          L)-, (2S,3Z)-/CN
E3      1 --> 3-PENTENOIC ACID, 5-(PHENYLTHIO)-/CN
E4      1      3-PENTENOIC ACID, 5-(PHENYLTHIO)-, METHYL ESTER, (3E)-/CN
E5      1      3-PENTENOIC ACID, 5-(PROPYLAMINO)-, ETHYL ESTER, (3E)-/CN
E6      1      3-PENTENOIC ACID, 5-(PROPYLAMINO)-, ETHYL ESTER, (3Z)-/CN
E7      1      3-PENTENOIC ACID, 5-(TETRAHYDRO-4,6-BIS((TRIMETHYLSILYL)OXY)
          -2-(3-((TRIMETHYLSILYL)OXY)-1-OCTENYL)-2H-PYRAN-3-YL)-, METH
          YL ESTER, (2R-(2A(1E,3S*)),3B(Z),4B,6A)
          )-/CN
E8      1      3-PENTENOIC ACID, 5-(TETRAHYDRO-4,6-DIHYDROXY-2-(3-HYDROXY-1
          ,5-OCTADIEN-1-YL)-2H-PYRAN-3-YL)-/CN
E9      1      3-PENTENOIC ACID, 5-(TETRAHYDRO-4,6-DIHYDROXY-2-(3-HYDROXY-1
          ,5-OCTADIENYL)-2H-PYRAN-3-YL)-/CN
E10     1      3-PENTENOIC ACID, 5-(TETRAHYDRO-4,6-DIHYDROXY-2-(3-HYDROXY-1
          -OCTEN-1-YL)-2H-PYRAN-3-YL)-/CN
E11     1      3-PENTENOIC ACID, 5-(TETRAHYDRO-4,6-DIHYDROXY-2-(3-HYDROXY-1
          -OCTENYL)-2H-PYRAN-3-YL)-/CN
E12     1      3-PENTENOIC ACID, 5-(TETRAHYDRO-4,6-DIHYDROXY-2-(3-HYDROXY-1
          -OCTENYL)-2H-PYRAN-3-YL)-, (2R-(2A(1E,3S*)),3B(Z),
          4B,6A))-/CN
```

=> e3

```
L10      1 "3-PENTENOIC ACID, 5-(PHENYLTHIO)-"/CN
```

=> d 110

```
L10 ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2010 ACS on STN
RN  80959-56-4  REGISTRY
ED  Entered STN: 16 Nov 1984
CN  3-Pentenoic acid, 5-(phenylthio)-  (CA INDEX NAME)
MF  C11 H12 O2 S
LC  STN Files:  BEILSTEIN*, CA, CAPLUS, CASREACT
          (*File contains numerically searchable property data)
```

PhS-CH2-CH=CH-CH2-CO2H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

309.74

309.96

FILE 'CAPLUS' ENTERED AT 05:43:31 ON 07 APR 2010

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 7 Apr 2010 VOL 152 ISS 15

FILE LAST UPDATED: 6 Apr 2010 (20100406/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2010

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2010

Caplus now includes complete International Patent Classification (IPC) reclassification data for the first quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l10

L11 1 L10

=> d l11 ti fbib abs

L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN

TI Regioselectivity of β -vinyl- β -propiolactone toward various nucleophiles

AN 1982:103582 CAPLUS <<LOGINID::20100407>>

DN 96:103582

OREF 96:17001a,17004a

TI Regioselectivity of β -vinyl- β -propiolactone toward various nucleophiles

AU Fujisawa, Tamotsu; Sato, Toshio; Takeuchi, Masashi

CS Chem. Dep. Resour., Mie Univ., Mie, 514, Japan

SO Chemistry Letters (1982), (1), 71-4

CODEN: CMLTAG; ISSN: 0366-7022

DT Journal

LA English
 OS CASREACT 96:103582
 AB Regioselectivity in the reaction of β -vinyl- β -propiolactone with various nucleophiles depends on the hard and soft acid and base (HSAB) principle. A hard base such as methoxide ion attacked the acyl carbon exclusively, while the nucleophilic attack of soft bases such as iodide and dialkyl cuprate preferred the terminal vinyl carbon to the β -carbon.

OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	6.60	316.56
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.85	-0.85

SESSION WILL BE HELD FOR 120 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 05:47:42 ON 07 APR 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
 SESSION RESUMED IN FILE 'CAPLUS' AT 05:50:04 ON 07 APR 2010
 FILE 'CAPLUS' ENTERED AT 05:50:04 ON 07 APR 2010
 COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	6.60	316.56
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.85	-0.85

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	10.10	320.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.85	-0.85

SESSION WILL BE HELD FOR 120 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 05:54:08 ON 07 APR 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SS\$PTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 06:05:27 ON 07 APR 2010
FILE 'CAPLUS' ENTERED AT 06:05:27 ON 07 APR 2010
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.10	320.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.85	-0.85

=> d his

(FILE 'HOME' ENTERED AT 05:07:01 ON 07 APR 2010)

FILE 'REGISTRY' ENTERED AT 05:07:13 ON 07 APR 2010

L1 STRUCTURE UPLOADED
L2 35 SEARCH L1 SSS SAM
L3 24701 SEARCH L1 SSS FULL
SAVE TEMP L3 MASTERSET/A
L4 STRUCTURE UPLOADED
L5 11 SEARCH L4 SSS SAM SUB=L3
L6 222 SEARCH L4 SSS FULL SUB=L3
SAVE TEMP L6 MSTRUNSATS/A
L7 STRUCTURE UPLOADED
L8 3 SEARCH L7 SSS SAM SUB=L6
L9 46 SEARCH L7 SSS FULL SUB=L6
E 3-PENTENOIC ACID, 5-(PHENYLTHIO)-/CN
L10 1 E3

FILE 'CAPLUS' ENTERED AT 05:43:31 ON 07 APR 2010

L11 1 L10

=> d l11 1 ti fbib abs it

L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN
TI Regioselectivity of β -vinyl- β -propiolactone toward various nucleophiles
AN 1982:103582 CAPLUS <<LOGINID::20100407>>
DN 96:103582
OREF 96:17001a,17004a
TI Regioselectivity of β -vinyl- β -propiolactone toward various nucleophiles
AU Fujisawa, Tamotsu; Sato, Toshio; Takeuchi, Masashi
CS Chem. Dep. Resour., Mie Univ., Mie, 514, Japan
SO Chemistry Letters (1982), (1), 71-4
CODEN: CMLTAG; ISSN: 0366-7022
DT Journal
LA English
OS CASREACT 96:103582
AB Regioselectivity in the reaction of β -vinyl- β -propiolactone with various nucleophiles depends on the hard and soft acid and base (HSAB)

principle. A hard base such as methoxide ion attacked the acyl carbon exclusively, while the nucleophilic attack of soft bases such as iodide and dialkyl cuprate preferred the terminal vinyl carbon to the β -carbon.

```
IT Substitution reaction, nucleophilic
    (of vinylpropiolactone, pentenoic acid derivs. from)
IT 7379-74-0
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (nucleophilic substitution of)
IT 62-53-3, reactions 67-56-1, reactions 108-98-5, reactions 123-75-1,
    reactions 124-41-4 693-03-8 930-69-8 7447-41-8, reactions
    7550-35-8 10377-51-2 26679-41-4 34762-98-6 54360-69-9 77090-33-6
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (nucleophilic substitution of, with vinylpropiolactone)
IT 4124-88-3P 38996-02-0P 43084-04-4P 80959-53-1P 80959-54-2P
    80959-55-3P 80959-56-4P 80959-57-5P 80959-58-6P
    80959-59-7P 80959-60-0P 80959-61-1P 80959-62-2P 80959-63-3P
    80959-64-4P 80967-14-2P 80967-15-3P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
```

```
=> 80959-56-4
    REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
```

```
L13 1 L12
```

```
=> display hitstr l13 1
```

```
L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN
IT 80959-56-4P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN 80959-56-4 CAPLUS
CN 3-Pentenoic acid, 5-(phenylthio)- (CA INDEX NAME)
```

PhS-CH2-CH=CH-CH2-CO2H

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.52	331.56
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.70

FILE 'REGISTRY' ENTERED AT 06:08:27 ON 07 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0
DICTIONARY FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

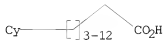
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 y2 bond pt vii genus.str

L14 STRUCTURE UPLOADED

=> d l14
L14 HAS NO ANSWERS
L14 STR



G1 O,N
G2 O,S,N,[@1-@2]

Structure attributes must be viewed using STN Express query preparation.

=> search l14 sss sam
 SAMPLE SEARCH INITIATED 06:09:08 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 80106 TO ITERATE

2.5% PROCESSED 2000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

3 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 1585257 TO 1618983
 PROJECTED ANSWERS: 1746 TO 3060

L15 3 SEA SSS SAM L14

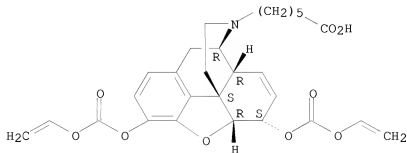
=> dscan

L16 0 DSCAN

=> d scan l15

L15 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Morphinan-17-hexanoic acid, 7,8-didehydro-4,5-epoxy-3,6-
 bis[(ethenyl)oxy]carbonyl]-, (5 α ,6 α)- (9CI)
 MF C28 H31 N O9

Absolute stereochemistry.



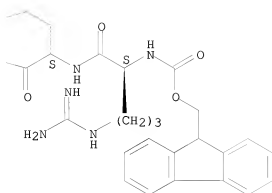
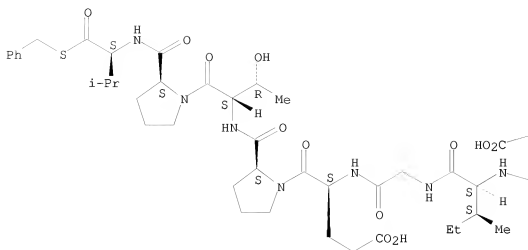
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L15 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN L-Valine, N2-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-arginyl-L- α -
 glutamyl-L-isoleucylglycyl-L- α -glutamyl-L-prolyl-L-threonyl-L-
 prolylthio-, 9-S-(phenylmethyl) ester
 SQL 9
 MF C65 H88 N12 O16 S

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

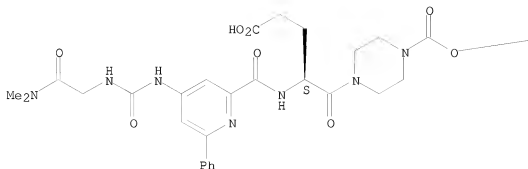


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

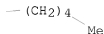
L15 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1-Piperazinepentanoic acid, γ -[[[4-[[[2-(dimethylamino)-2-oxoethyl]amino]carbonyl]amino]-6-phenyl-2-pyridinyl]carbonyl]amino]- δ -oxo-4-[[pentyloxy]carbonyl]-, (γ S)-
 MF C32 H43 N7 O8

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l14 sss full
 FULL SEARCH INITIATED 06:10:54 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 1603430 TO ITERATE

72.8% PROCESSED	1167273 ITERATIONS	1338 ANSWERS
93.5% PROCESSED	1498657 ITERATIONS	1789 ANSWERS
99.0% PROCESSED	1587265 ITERATIONS	1810 ANSWERS
100.0% PROCESSED	1603430 ITERATIONS	1810 ANSWERS
SEARCH TIME: 00.01.06		

L17 1810 SEA SSS FUL L14

=> d scan

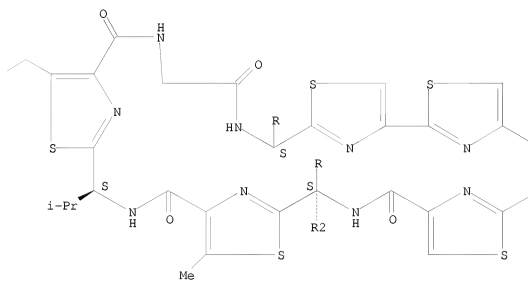
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Cyclohexanepentanoic acid, 1-carboxy-4-[[[(4-carboxybutyl)[2-
 [(11S,18S,28S)-10,11,17,18,23,24,25,26,27,28-decahydro-28-[(S)-
 hydroxyphenylmethyl]-21-(methoxymethyl)-14-methyl-11-[2-(methylamino)-2-
 oxoethyl]-18-(1-methylethyl)-9,16,23,26-tetraoxo-9H,16H-
 8,5:15,12:22,19:32,29:36,33-pentanitrilo-5H,29H,33H-pyrido[3,2-
 al][1,11,18,25,31,4,7,14,21]pentathiatetraazacyclotetratriacontin-2-yl]-4-
 thiazolyl]amino]carbonyl]oxy]-, cis-
 MF C65 H71 N13 O15 S6

Absolute stereochemistry.

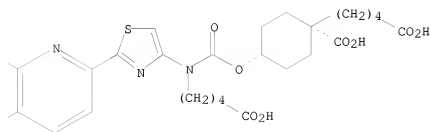
PAGE 1-B

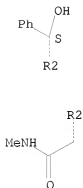
MeO

PAGE 1-C



PAGE 1-D

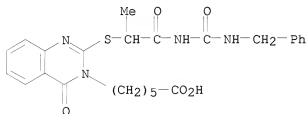




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

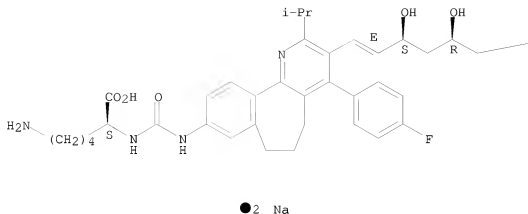
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3(4H)-Quinazolinehexanoic acid, 2-[[1-methyl-2-oxo-2-
 [[[phenylmethyl)amino]carbonyl]amino]ethyl]thio]-4-oxo-
 MF C28 H28 N4 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 6-Heptenoic acid, 7-[9-[[[(1S)-5-amino-1-
 carboxypentyl]amino]carbonyl]amino]-4-(4-fluorophenyl)-6,7-dihydro-2-(1-
 methylethyl)-5H-benzo[6,7]cyclohepta[1,2-b]pyridin-3-yl]-3,5-dihydroxy-,
 sodium salt (1:2), (3R,5S,6E)-
 MF C37 H45 F N4 O7 . 2 Na

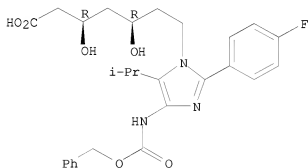
Absolute stereochemistry.
 Double bond geometry as shown.



—CO₂H

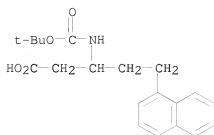
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1H-Imidazole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-
 5-(1-methylethyl)-4-[[[(phenylmethoxy)carbonyl]amino]-, (βR,δR)-
 MF C27 H32 F N3 O6
 CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1-Naphthalenepentanoic acid, β-[[[(1,1-dimethylethoxy)carbonyl]amino]-
 MF C20 H25 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN L-Argininamide, N2-(4-fluorobenzoyl)-L-arginyl-L-arginyl-3-(2-naphthalenyl)-L-alanyl-L-cysteinyl-L-tyrosyl-N5-(aminocarbonyl)-L-ornithyl-L-lysyl-D-α-glutamyl-L-prolyl-L-tyrosyl-L-arginyl-N5-(aminocarbonyl)-L-ornithyl-L-cysteinyl-

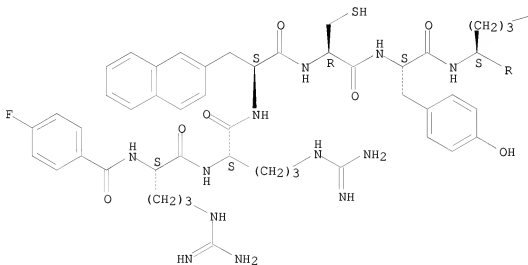
SOL 14

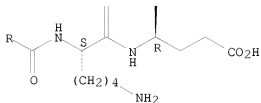
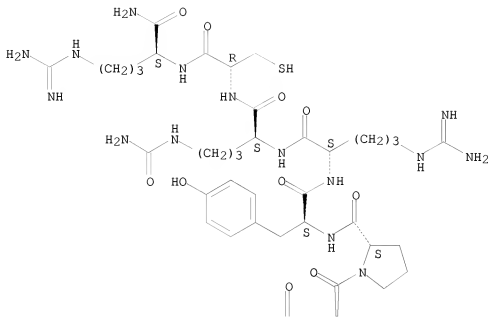
MF C96 H141 F N32 O21 S2

RELATED SEQUENCES AVAILABLE WITH SEOLINK

Absolute stereochemistry.

PAGE 1-A

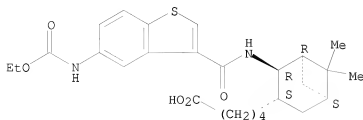




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Bicyclo[3.1.1]heptane-3-pentanoic acid,
 2-[[[5-[(ethoxycarbonyl)amino]benzo[b]thien-3-yl]carbonyl]amino]-6,6-
 dimethyl-, (1R,2R,3S,5S)-
 MF C26 H34 N2 O5 S

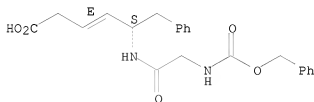
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[2-
 [[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, (3E,5S)-
 MF C22 H24 N2 O5

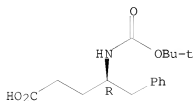
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

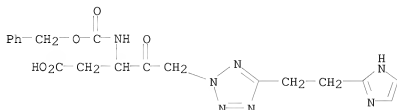
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepentanoic acid, γ -[[[(1,1-dimethylethoxy)carbonyl]amino]-,
 (γ R)-
 MF C16 H23 N O4

Absolute stereochemistry. Rotation (-).



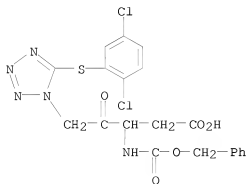
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2H-Tetrazole-2-pentanoic acid, 5-[2-(1H-imidazol-2-yl)ethyl]-γ-oxo-
 β-[[[(phenylmethoxy)carbonyl]amino]-, monohydrochloride (9CI)
 MF C19 H21 N7 O5 . C1 H



● HCl

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1H-Tetrazole-1-pentanoic acid, 5-[(2,5-dichlorophenyl)thio]-γ-oxo-
 β-[[[(phenylmethoxy)carbonyl]amino]-
 MF C20 H17 Cl2 N5 O5 S



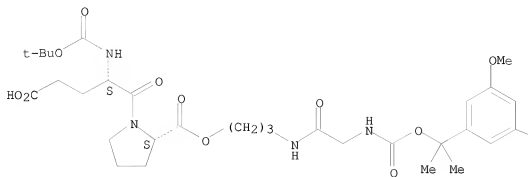
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN L-Proline, N-[(1,1-dimethylethoxy)carbonyl]-L-α-glutamyl-,
 2-[3-[[[1-(3,5-dimethoxyphenyl)-1-methylethoxy]carbonyl]amino]acetyl]amino]propyl] ester (9CI)
 MF C32 H48 N4 O12

Absolute stereochemistry.

PAGE 1-A

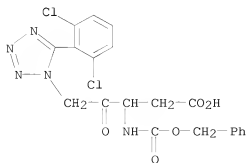


PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

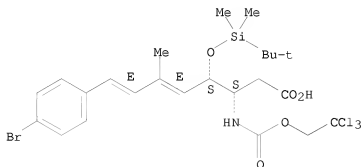
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1H-Tetrazole-1-pentanoic acid, 5-(2,6-dichlorophenyl)-γ-oxo-β-
 [[(phenylmethoxy)carbonyl]amino]-
 MF C20 H17 Cl2 N5 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

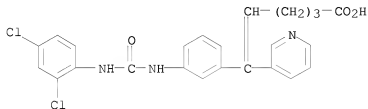
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5,7-Octadienoic acid, 8-[(4-bromophenyl)-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-3-[[[(2,2,2-trichloroethoxy)carbonyl]amino]-, [S-[R*,R*-(E,E)]]- (9CI)
 MF C24 H33 Br Cl3 N O5 Si

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Hexenoic acid, 6-[3-[[[(2,4-dichlorophenyl)amino]carbonyl]amino]phenyl]-6-(3-pyridinyl)-
 MF C24 H21 Cl2 N3 O3

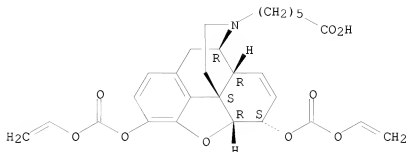


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Morphinan-17-hexanoic acid, 7,8-didehydro-4,5-epoxy-3,6-bis[[[ethenyloxy]carbonyl]oxy]-, (5a,6a)- (9CI)

MF C28 H31 N O9

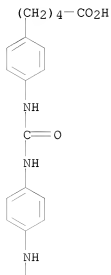
Absolute stereochemistry.

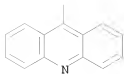


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenepentanoic acid, 4-[[[4-(9-acridinylamino)phenyl]amino]carbonyl]amino]-
MF C31 H28 N4 O3
CI COM

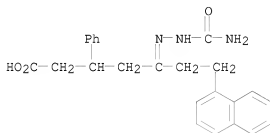
PAGE 1-A





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

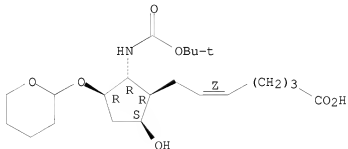
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1-Naphthaleneheptanoic acid, 8-[2-(aminocarbonyl)hydrazinylidene]-
 β-phenyl-
 MF C24 H25 N3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

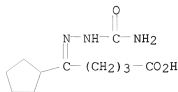
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 5-Heptenoic acid, 7-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]-5-hydroxy-3-
 [(tetrahydro-2H-pyran-2-yl)oxy]cyclopentyl]-,
 [1R-[1α(Z),2β,3α,5α]]- (9CI)
 MF C22 H37 N O7

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

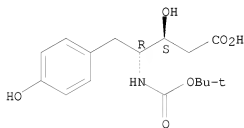
L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Cyclopentanepentanoic acid, δ -[2-(aminocarbonyl)hydrazinylidene]-
 MF C11 H19 N3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L17 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN D-erythro-Pentonic acid, 2,4,5-trideoxy-4-[(1,1-dimethylethoxy)carbonyl]amino]-5-(4-hydroxyphenyl)-
 MF C16 H23 N O6

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp l17 y2bondmstrset/a
 Y2BONDMSTRSET/A IS NOT A VALID SAVED NAME
 Enter the name you wish to use for the saved query,
 answer set, or L-number list. The name must:

1. Begin with a letter,
2. Have 1-12 characters,
3. Contain only letters (A-Z) and numbers (0-9),
4. End with /Q for a query (search profile, structure, or screen set), /A for an answer set, or /L for an L-number list.
5. Not already be in use as a saved name,
6. Not be END, SAV, SAVE, SAVED
7. Not have the form of an L-number (Lnnn).

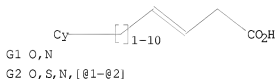
ENTER NAME OR (END):end

=> save temp l17 y2bondmstr/a
ANSWER SET L17 HAS BEEN SAVED AS 'Y2BONDMSTR/A'

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 unsatsy2bond.str

L18 STRUCTURE UPLOADED

=> d l18
L18 HAS NO ANSWERS
L18 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l18 sss sam subset=l17
SAMPLE SUBSET SEARCH INITIATED 06:20:05 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):	ONLINE	**COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):	5 TO	234
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):	2 TO	124

L19 2 SEA SUB=L17 SSS SAM L18

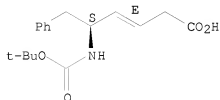
=> dscan
L20 0 DSCAN

=> d scan l19

L19 2 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-,

(3E,5S)-
 MF C17 H23 N O4
 CI COM

Absolute stereochemistry.
 Double bond geometry as shown.

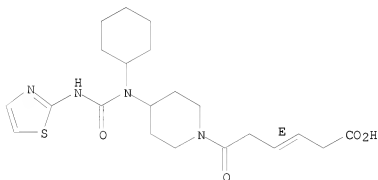


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L19 2 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-[4-(cyclohexyl[(2-thiazolylamino)carbonyl]amino)-1-
 piperidinyl]-6-oxo-, (3E)-
 MF C21 H30 N4 O4 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e 3-Hexenoic acid, 5-(((1,1-dimethylethoxy)carbonyl)amin)]-6-phenyl-, /cn
 E1 1 3-HEXENOIC ACID, 5-(((5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL)OXY)CARBONYL)AMINO)-2-(2-METHYLPROPYL)-, (1R-(1-ALPHA-(2S*,3E,5R*),2B,5A))- /CN
 E2 1 3-HEXENOIC ACID, 5-(((5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL)OXY)CARBONYL)AMINO)-2-(2-METHYLPROPYL)-, METHYL EST

ER, (1R-(1A(2S*,3E,5R*),2B,5A))-/CN
E3 0 --> 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-6-PHENYL-, /CN
E4 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (1,1-DIMETHYLETHYL)DIPHENYLSILYL ESTER, (R-(E))-/CN
E5 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (2,2-DIMETHYL-1-OXOPROPOXY)METHYL ESTER, (R)-/CN
E6 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (R-(E))-/CN
E7 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (S-(E))-/CN
E8 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, METHYL ESTER, (R-(E))-/CN
E9 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, METHYL ESTER, (S-(E))-/CN
E10 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-2,4-DIMETHYL-, METHYL ESTER, (S-(R*,S*-(E)))-/CN
E11 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-2-(1,1-DIMETHYLETHYL)-4-METHYL-, METHYL ESTER, (2S,3E,5S)-/CN
E12 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-2-(1,1-DIMETHYLETHYL)-6-(1-(2,4,6-TRIMETHYLPHENYL)SULFONYL)-1H-INDOL-3-YL-, METHYL ESTER, (2R,3E,5S)-/CN

=> e 3-Hexenoic acid, 5-(((1,1-dimethylethoxy)carbonyl)amino)]-6-phenyl-, /cn
E1 1 3-HEXENOIC ACID, 5-((((5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL)OXY)CARBONYL)AMINO)-2-(2-METHYLPROPYL)-, (1R-(1. ALP HA, (2S*,3E,5R*),2B,5A))-/CN
E2 1 3-HEXENOIC ACID, 5-((((5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL)OXY)CARBONYL)AMINO)-2-(2-METHYLPROPYL)-, METHYL ESTER, (1R-(1A(2S*,3E,5R*),2B,5A))-/CN
E3 0 --> 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-6-PHENYL-, /CN
E4 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (1,1-DIMETHYLETHYL)DIPHENYLSILYL ESTER, (R-(E))-/CN
E5 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (2,2-DIMETHYL-1-OXOPROPOXY)METHYL ESTER, (R)-/CN
E6 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (R-(E))-/CN
E7 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, (S-(E))-/CN
E8 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, METHYL ESTER, (R-(E))-/CN
E9 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-, METHYL ESTER, (S-(E))-/CN
E10 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-2,4-DIMETHYL-, METHYL ESTER, (S-(R*,S*-(E)))-/CN
E11 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-2-(1,1-DIMETHYLETHYL)-4-METHYL-, METHYL ESTER, (2S,3E,5S)-/CN
E12 1 3-HEXENOIC ACID, 5-(((1,1-DIMETHYLETHOXY)CARBONYL)AMINO)-2-(1,1-DIMETHYLETHYL)-6-(1-(2,4,6-TRIMETHYLPHENYL)SULFONYL)-1H-INDOL-3-YL-, METHYL ESTER, (2R,3E,5S)-/CN

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
CA SUBSCRIBER PRICE

SINCE FILE ENTRY	TOTAL SESSION
214.30	545.86
SINCE FILE ENTRY	TOTAL SESSION
0.00	-1.70

FILE 'CAPLUS' ENTERED AT 06:23:09 ON 07 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 7 Apr 2010 VOL 152 ISS 15
FILE LAST UPDATED: 6 Apr 2010 (20100406/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2010

Caplus now includes complete International Patent Classification (IPC) reclassification data for the first quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l19

L21 13 L19

=> d l21 1-13 ti

L21 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI Preparation of dicycloalkyl thiazolyl ureas as glucokinase activators

L21 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI Preparation of dicycloalkyl thiazolyl ureas as glucokinase activators

L21 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI E-Olefin Dipeptide Isostere Incorporation into a Polypeptide Backbone Enables Hydrogen Bond Perturbation: Probing the Requirements for Alzheimer's Amyloidogenesis

L21 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI Novel synthesis of a Phe-Gly E-alkene dipeptide isostere

L21 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI Stereoselective Epoxidation of Phe-Gly and Phe-Phe Vinyl Isosteres

L21 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI Novel L-Phe-Gly mimetics

L21 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
TI Synthesis and biological activities of bradykinin analogs with $\Psi(E,CH:CH)$ and $\Psi(CH_2NH)$ isosteric peptide bond replacements

L21 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

TI Monitoring of the chiral purity of $\Psi(E,CH:CH)$ dipeptides using 2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl isothiocyanate

L21 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Preparation of retroviral protease binding peptides

L21 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Preparation of retroviral protease-inhibiting peptides and pharmaceutical compositions containing them

L21 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Renin inhibitors containing isosteric replacements of the amide bond connecting the P3 and P2 sites

L21 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Preparation of peptides as renin inhibitors

L21 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Nonhydrolyzable tripeptide analogs as angiotensin-converting enzyme inhibitors

=> d l21 8-13 ti fbib abs

L21 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Monitoring of the chiral purity of $\Psi(E,CH:CH)$ dipeptides using 2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl isothiocyanate
 AN 1991:515076 CAPLUS <<LOGINID::20100407>>
 DN 115:115076
 OREF 115:19753a,19756a
 TI Monitoring of the chiral purity of $\Psi(E,CH:CH)$ dipeptides using 2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl isothiocyanate
 AU Devadder, S.; Couder, J.; Jaspers, H.; Ceusters, M.; Tourwe, D.; Van Binst, G.
 CS Vrije Univ. Brussel, Brussels, B-1050, Belg.
 SO Bulletin des Societes Chimiques Belges (1991), 100(5), 407-9
 CODEN: BSCBAG; ISSN: 0037-9646
 DT Journal
 LA English
 AB Condensation of α -amino aldehydes Boc-X-H (Boc = Me₃CO₂C; X = Phe, Ala, Pro, 4-fluorophenylalanine) with Ph₃P+CH₂C.tplbond.CSiMe₃ gave enynes, e.g. (E)-Boc-L-NHCH₂CH:CHC.tplbond.CSiMe₃ (R = CH₂Ph, Me, CH₂C₆H₄F-4), which underwent hydroboration and oxidation to give the title dipeptide isosteres (E)-Boc-L-NHCH₂CH:CHCH₂CO₂H (I). The optical purities of I were checked by deblocking and condensation with the title isothiocyanate. Excellent baseline resolution was obtained for the derivs. of I while the corresponding adduct of (E)-Boc-L-NHCH₂CH:CHCH(CH₂Ph)CO₂H was only partially resolved.

L21 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Preparation of retroviral protease binding peptides
 AN 1991:240604 CAPLUS <<LOGINID::20100407>>
 DN 114:240604
 OREF 114:40421a,40424a
 TI Preparation of retroviral protease binding peptides
 IN Dreyer, Geoffrey Bainbridge; Huffman, William Francis; Meek, Thomas Downing; Metcalf, Brian Walter; Moore, Michael Lee
 PA SmithKline Beckman Corp., USA
 SO PCT Int. Appl., 214 pp.
 CODEN: PIXXD2
 DT Patent

LA English
FAN.CNT 2

PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
PI	WO 9000399	A1	19900125	WO 1989-US2972	19890707
	W: AU, DK, FI, HU, JP, KR, NO				
	AU 8939644	A	19900205	US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				AU 1989-39644	19890707
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				WO 1989-US2972	A 19890707
	ZA 8905174	A	19900328	ZA 1989-5174	19890707
				US 1988-216178	A 19880708
	JP 03505875	T	19911219	JP 1989-507665	19890707
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				WO 1989-US2972	W 19890707
	HU 58764	A2	19920330	HU 1989-4124	19890707
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
	DK 9100026	A	19910306	DK 1991-26	19910107
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				WO 1989-US2972	A 19890707
	NO 9100053	A	19910307	NO 1991-53	19910107
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				WO 1989-US2972	W 19890707
	NO 9200318	A	19910307	NO 1992-318	19920123
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				WO 1989-US2972	W 19890707
				NO 1991-53	A1 19910107
	NO 9200319	A	19910307	NO 1992-319	19920123
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				US 1989-374326	A 19890629
				WO 1989-US2972	W 19890707
				NO 1991-53	A1 19910107

PATENT FAMILY INFORMATION:

PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
FAN	1990:553045				
PI	EP 352000	A2	19900124	EP 1989-306995	19890710
	EP 352000	A3	19910717		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8905174	A	19900328	US 1988-216178	A 19880708
				US 1989-321937	A 19890310
				ZA 1989-5174	19890707
				US 1988-216178	A 19880708
	CN 1039596	A	19900214	CN 1989-104699	19890708
				US 1988-216178	A 19880708
				US 1989-321937	A 19890310

OS MARPAT 114:240604
 AB The peptides ABQaCbCdMwXeYZ [I; A = H, Boc, Cbz, etc.; B = L- or D-amino acid(s), β -Ala, or covalent bond; Q = D- or L-Ser, -Thr, -Asp, etc.; C, D = Ala, β -Ala, Arg, Gly, etc.; W = Pro or Δ^3 -dehydro-Pro; X = Ala, Gly, Ile, Leu, etc.; Y = L- or D-amino acid(s) or covalent bond; Z = (modified) CO₂H of amino acid residue Y, e.g. CONRR1, CO₂R1, CH₂OH; M = NHCHQ1CO, NHCHR2R3, Phe (4'-R4); R, R1 = H, alkyl; R2 = alkyl, alkylthioalkyl, alkoxyalkyl, etc.; R3 = (CH₂)_n, CO(CH₂)_mCO, etc.; R4 = H, halo, OR, NO₂, NH₂; Q1 = cyclohexylmethyl; a, b, c, d, e = 0, 1; n = 1, 2; m = 0-3] and I salts are prepared as mimics of the retrovirus protease polypeptide substrate. I bind to the viral proteases and are therefore useful for protease assay and therapeutical purposes. (2S)-N-[2-(2-N-tert-Butyloxycarbonyl)amino-3-phenylpropyl]-L-proline (preparation given) was coupled to Val-Val-BHA resin, using DCC 1-hydroxybenzotriazole in CH₂Cl₂-DMF mixture. Peptide cleavage from the resin was carried out with HF and anisole, to give 2-(serylglutaminylasparaginyl)amino-3-phenylpropylpropylvalylvalinamide (II). II inhibited recombinant human immunodeficiency virus protease with an inhibition constant (K_i) of 1 μ M.

OSC.G 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
 RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Preparation of retroviral protease-inhibiting peptides and pharmaceutical compositions containing them
 AN 1990:553045 CAPLUS <<LOGINID::20100407>>
 DN 113:153045
 OREF 113:26035a,26038a
 TI Preparation of retroviral protease-inhibiting peptides and pharmaceutical compositions containing them
 IN Dreyer, Geoffrey Bainbridge; Huffman, William Francis; Meek, Thomas Dowling; Metcalf, Brian Walter; Moore, Michael Lee
 PA SmithKline Beckman Corp., USA
 SO Eur. Pat. Appl., 118 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 352000	A2	19900124	EP 1989-306995	19890710
EP 352000	A3	19910717		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 8905174	A	19900328	US 1988-216178	A 19880708
			US 1989-321937	A 19890310
			ZA 1989-5174	19890707
			US 1988-216178	A 19880708
CN 1039596	A	19900214	CN 1989-104699	19890708
			US 1988-216178	A 19880708
			US 1989-321937	A 19890310

PATENT FAMILY INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9000399	A1	19900125	WO 1989-US2972	19890707
W: AU, DK, FI, HU, JP, KR, NO				
			US 1988-216178	A 19880708
			US 1989-321937	A 19890310
			US 1989-374326	A 19890629
AU 8939644	A	19900205	AU 1989-39644	19890707

			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
			WO 1989-US2972	A	19890707
ZA 8905174	A	19900328	ZA 1989-5174		19890707
			US 1988-216178	A	19880708
JP 03505875	T	19911219	JP 1989-507665		19890707
			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
			WO 1989-US2972	W	19890707
HU 58764	A2	19920330	HU 1989-4124		19890707
			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
DK 9100026	A	19910306	DK 1991-26		19910107
			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
			WO 1989-US2972	A	19890707
NO 9100053	A	19910307	NO 1991-53		19910107
			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
			WO 1989-US2972	W	19890707
NO 9200318	A	19910307	NO 1992-318		19920123
			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
			WO 1989-US2972	W	19890707
			NO 1991-53	A1	19910107
NO 9200319	A	19910307	NO 1992-319		19920123
			US 1988-216178	A	19880708
			US 1989-321937	A	19890310
			US 1989-374326	A	19890629
			WO 1989-US2972	W	19890707
			NO 1991-53	A1	19910107
OS	MARPAT 113:153045				
AB	<p>A-B-(Q)a-(C)b-(D)c-M-(W)d-(X)e-Y-Z [I; A = H, protecting group, (protected) amino, alkanamido, etc.; B = D- or L-amino acid residue, e.g., β-Ala, bond; C, D = Glx, Asx, Ala, β-Ala, Arg, Gly, Ile, Leu, Lys, Ser, Thr, Val, Met, His; Asx = Asp, Asn; Glx = Glu, Gln; Q = D- or L-amino acid residue, e.g.; Ser, Thr, Asp, His, Cys, Arg, Ala; W = Pro, dehydro-Pro; X = Ala, Gly, Ile, Leu, Val, Met, Lys, Glx, Asx; Y = D- or L-amino acid residue(s), bond; Z = CO₂H, alkoxycarbonyl, (substituted) amino, etc.; a-e = 0, 1, however, c and e may not simultaneously be 0; M = Cha, (substituted) Phe, alkylamino] and their pharmaceutically acceptable salts were prepared Many I, e.g., Ac-Ser-Gln-Ser-Tyr-Pro-Val-Val-NH₂, were prepared by solid-phase or solution synthesis.</p> <p>2-(Acetylserylglutaminylasparaginy)amino-3-phenylpropylprolylvalylvalinamide (preparation given) showed an inhibition constant K_i of 14 μM in vitro against rHIV protease. Many pharmaceutical dosage forms containing I were formulated.</p>				
OSC.G	21	THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)			
L21	ANSWER 11 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN				
TI	Renin inhibitors containing isosteric replacements of the amide bond connecting the P3 and P2 sites				
AN	1990:56684 CAPLUS <<LOGINID::20100407>>				
DN	112:56684				
OREF	112:9759a,9762a				

TI Renin inhibitors containing isosteric replacements of the amide bond connecting the P3 and P2 sites
 AU Kaltenbronn, James S.; Hudspeth, J. P.; Lunney, E. A.; Michniewicz, B. M.; Nicolaides, E. D.; Repine, J. T.; Roark, W. H.; Stier, M. A.; Tinney, F. J.; et al.
 CS Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
 SO Journal of Medicinal Chemistry (1990), 33(2), 838-45
 CODEN: JMCMAR; ISSN: 0022-2623
 DT Journal
 LA English
 OS CASREACT 112:56684
 AB Renin inhibitors having 13 different isosteres connecting the P3 and P2 positions have been prepared. Synthetic routes and in vitro activity exhibited by these compds. are discussed. The two most potent compds. contained the hydroxyethylene isostere.
 OSC.G 43 THERE ARE 43 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)

L21 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

TI Preparation of peptides as renin inhibitors

AN 1989:439861 CAPLUS <<LOGINID::20100407>>

DN 111:39861

OREF 111:6805a,6808a

TI Preparation of peptides as renin inhibitors

IN Hudspeth, James P.; Kaltenbronn, James S.; Lunney, Elizabeth A.; Repine, Joseph T.; Roark, W. Howard; Stier, Michael A.; Tinney, Francis J.; Woo, Peter W. K.; Nicolaides, Ernest D.

PA Warner-Lambert Co., USA

SO U.S., 64 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4743585	A	19880510	US 1986-920330	19861121
WO 8803927	A2	19880602	WO 1987-US2820	19871021
WO 8803927	A3	19880811		
W: AU, BB, BG, BR, DK, FI, HU, JP, KP, KR, LK, MC, MG, MW, NO, RO, SD, SU, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8783361	A	19880616	US 1986-920330	A1 19861121
			AU 1987-83361	19871021
			US 1986-920330	A 19861121
			WO 1987-US2820	A 19871021

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LUS DISPLAY FORMAT

OS MARPAT 111:39861

AB R-X-An-Y-Bn-T-Cn-W-Dn-V-En-U [I; n = 0, 1, the compound must contain ≥ 1 link where n = 1; R = CO₂Me₃, CO₂CH₂Ph, valeryl, isovaleryl, isobutyryl, Bz, HO₂C(CH₂)₃CO, Me₃CCO; X = Phe, Trp, cyclohexyl-Ala, 1-naphthyl-Ala, homo-Phe, Phe(Me₅), Val, Ile, Leu; Y = bond, Phe, His, His(CH₂CO₂CH₂Ph), Gly, phenyl-Gly, Leu, Val, Ile, Orn, Orn(phthaloyl), Arg, Arg(NO₂); T = sta, benzidine or cyclotene residue, Leu, cyclohexyl-Ala, Phe; W = bond, Leu, Gly, Ile; V = bond, Leu, Ile; U = NHCH₂Ph, NHCH₂C₆H₄(CH₂NHCO₂CH₂Ph)-3, NH₂, OMe, OEt, etc.; A = CH₂NH, CH₂NOH, CH₂S, CH₂SO, CH:CH, CH(OH)CH₂, CH(OH)CH(OH), COCH₂, etc.; B = CH₂NH; C = CH₂NH, CH(OH)CH₂, CH(OH)CH:CHCH₂; D = CH₂NH; E = CH₂NH, CH₂NHCO₂CH₂Ph], useful for treatment of renin-associated hypertension and hyperaldosteronism, were prepared. A solution of 0.5 H-Sta-Ala-Sta-NHCH₂Ph, 0.5 [S-(E)]-5-[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-3-hexenoic acid, and 0.5 mmol 1-hydroxybenzotriazole in DMF was cooled in ice and treated

with a solution of dicyclohexylcarbodiimide in DMF. After 1 h at 0°, the mixture was stirred at room temperature overnight to give 240 mg [5S-[5R,6R,9R,13R,14R-(E),20R]]-20-benzyl-3,8,11,16-tetraoxo-1-phenyl-2,7,10,15,21-pentaazadocos-18-en-22-oic acid 1,1-dimethylethyl ester [BOC-Phe[CH=CH]Gly-Sta-Ala-Sta-NHCH2Ph] (BOC = CO2CMe3). I in vitro inhibited renin with IC50 of 1.4 + 10-8 to 6.3 + 10-5 M.

OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

TI Nonhydrolyzable tripeptide analogs as angiotensin-converting enzyme inhibitors

AN 1982:402688 CAPLUS <<LOGINID::20100407>>

DN 97:2688

OREF 97:551a,554a

TI Nonhydrolyzable tripeptide analogs as angiotensin-converting enzyme inhibitors

AU Natarajan, S.; Condon, M. E.; Nakane, M.; Reid, J.; Gordon, E. M.; Cushman, D. W.; Ondetti, M. A.

CS Squibb Inst. Med. Res., Princeton, NJ, 08540, USA

SO Pept.: Synth., Struct., Funct., Proc. Am. Pept. Symp., 7th (1981), 429-33. Editor(s): Rich, Daniel H.; Gross, Erhard. Publisher: Pierce Chem. Co., Rockford, Ill.

CODEN: 47LMAO

DT Conference

LA English

AB The hydrolyzable amide bond of suitable tripeptide substrates for angiotensin-converting enzyme (I) was modified to produce nonhydrolyzable moieties which acted as inhibitors. Modification of the amide bond to a ketomethylene moiety gave rise to the most potent inhibitor studied (II; PhCONHCH(CH2Ph)COCH2CH2CO-Pro-OH), with an I50 value (concentration for 50% of maximum inhibition) of 0.01 µM. The increased potency of II is apparently caused by resistance to hydrolysis by I, the specific interaction of the C:O group and functional residues of the active site of I, or a combination of both. The nonhydrolyzable analogs synthesized retained a number of the I-binding functional groups of the peptide substrate: C-terminal carboxyl, ultimate amide bond, and side chains for secondary interactions. Modification of the amide bond to a secondary amine to produce reduction analogs yielded compds. which retained tetrahedral N in the transition state. Replacement of the amide bond with olefinic groups or ketomethylene groups (other than II) produced inhibitors of much poorer potency than II. An analog with a CH2-S replacing the amide was also synthesized.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
42.27	588.13

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-5.10	-6.80

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 06:27:11 ON 07 APR 2010

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0
DICTIONARY FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> search l18 sss full subset=l17
FULL SUBSET SEARCH INITIATED 06:27:36 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 90 TO ITERATE
```

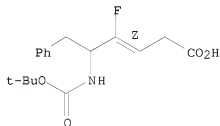
```
100.0% PROCESSED          90 ITERATIONS          39 ANSWERS
SEARCH TIME: 00.00.01
```

```
L22          39 SEA SUB=L17 SSS FUL L18
```

```
=> d scan
```

```
L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
, (Z)- (9CI)
MF C17 H22 F N O4
```

Double bond geometry as shown.



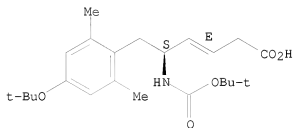
****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

```
L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-
dimethylethoxy)-2,6-dimethylphenyl]-, [S-(E)]- (9CI)
MF C23 H35 N O5
```

Absolute stereochemistry.

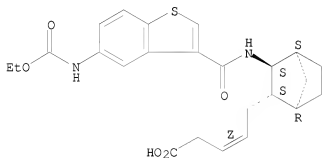
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[(1R,2S,3S,4S)-3-[[[5-
 [(ethoxycarbonyl)amino]benzo[b]thien-3-
 yl]carbonyl]amino]bicyclo[2.2.1]hept-2-yl]-, (3Z)-
 MF C24 H28 N2 O5 S

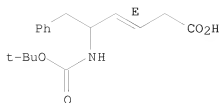
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-, (E)-
 (9CI)
 MF C17 H23 N O4

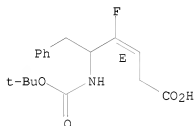
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[1-oxo-3-phenyl-2-
 , (E)- (9CI)
 MF C17 H22 F N O4

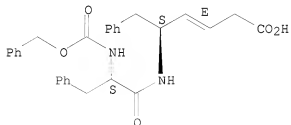
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[1-oxo-3-phenyl-2-
 [[(phenylmethoxy)carbonyl]amino]propyl]amino]-6-phenyl-, [S-[R*,R*-(E)]]-
 (9CI)
 MF C29 H30 N2 O5

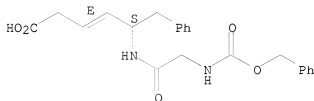
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[2-
 [[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, (3E,5S)-
 MF C22 H24 N2 O5

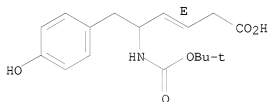
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(4-
 hydroxyphenyl)-, (E)- (9CI)
 MF C17 H23 N O5

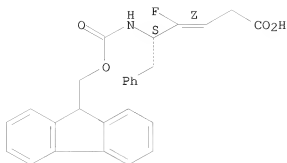
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-
 phenyl-, (3Z,5S)-
 MF C27 H24 F N O4

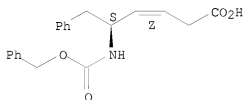
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[[(phenylmethoxy)carbonyl]amino]-, (3Z,5S)-
 MF C20 H21 N O4

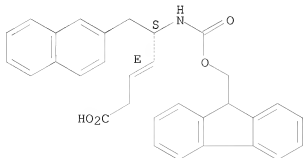
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-6-(2-naphthalenyl)-, (3E,5S)-
 MF C31 H27 N O4

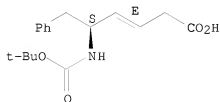
Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-,
(3E,5S)-
MF C17 H23 N O4
CI COM

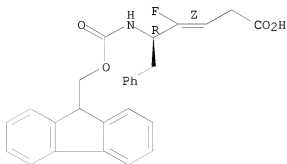
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-
phenyl-, [R-(Z)]- (9CI)
MF C27 H24 F N O4

Absolute stereochemistry.
Double bond geometry as shown.

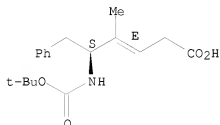


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-6-phenyl-

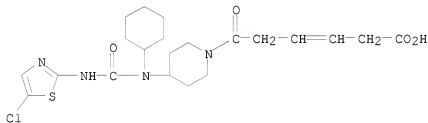
, [S-(E)]- (9CI)
 MF C18 H25 N O4

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

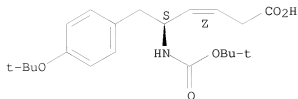
L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-[4-[[[(5-chloro-2-thiazolyl)amino]carbonyl]cyclohexylamino]-1-piperidinyl]-6-oxo-
 MF C21 H29 Cl N4 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-dimethylethoxy)phenyl]-, [S-(Z)]- (9CI)
 MF C21 H31 N O5
 CI COM

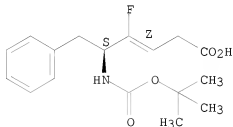
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
 , [S-(Z)]- (9CI)
 MF C17 H22 F N O4

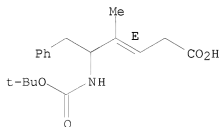
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-6-phenyl-
 , (E)- (9CI)
 MF C18 H25 N O4

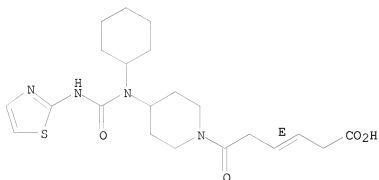
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-[4-[cyclohexyl[(2-thiazolylamino)carbonyl]amino]-1-
 piperidinyl]-6-oxo-, (3E)-
 MF C21 H30 N4 O4 S

Double bond geometry as shown.

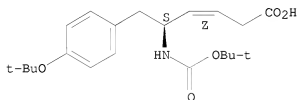


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

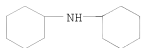
L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-
 dimethylethoxy)phenyl]-, [S-(Z)]-, compd. with N-cyclohexylcyclohexanamine
 (1:1) (9CI)
 MF C21 H31 N O5 . C12 H23 N

CM 1

Absolute stereochemistry.
 Double bond geometry as shown.

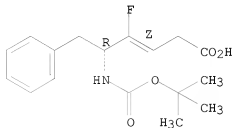


CM 2



L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
 , [R-(Z)]- (9CI)
 MF C17 H22 F N O4

Absolute stereochemistry.
 Double bond geometry as shown.

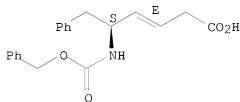


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[[(phenylmethoxy)carbonyl]amino]-, [S-(E)]-
 (9CI)
 MF C20 H21 N O4

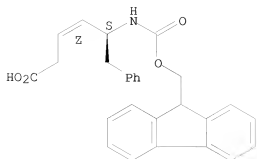
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-6-phenyl-,
 (3Z,5S)-
 MF C27 H25 N O4

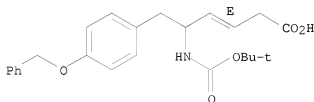
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-
 (phenylmethoxy)phenyl]-, (3E)-
 MF C24 H29 N O5

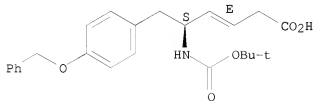
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-
 (phenylmethoxy)phenyl]-, [S-(E)]- (9CI)
 MF C24 H29 N O5

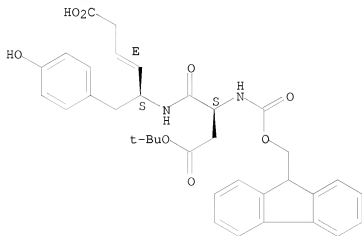
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(2S)-4-(1,1-dimethylethoxy)-2-[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1,4-dioxobutyl]amino]-6-(4-hydroxyphenyl)-, (3E,5S)-
 MF C35 H38 N2 O8

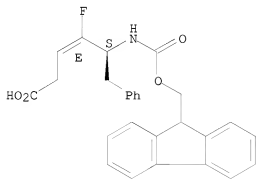
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, (3E,5S)-
 MF C27 H24 F N O4

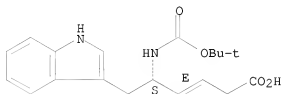
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(1H-indol-3-yl)-
 , [S-(E)]- (9CI)
 MF C19 H24 N2 O4

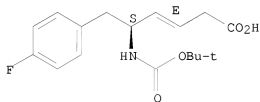
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(4-
 fluorophenyl)-, [S-(E)]- (9CI)
 MF C17 H22 F N O4
 CI COM

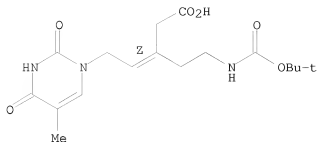
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-3-
 [[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (3Z)-
 MF C17 H25 N3 O6

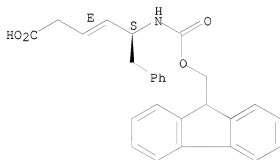
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-6-phenyl-,
 (3E,5S)-
 MF C27 H25 N O4

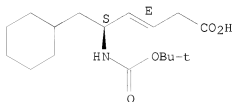
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-cyclohexyl-5-[[[(1,1-dimethylethoxy)carbonyl]amino]-,
 [S-(E)]- (9CI)
 MF C17 H29 N O4

Absolute stereochemistry.
 Double bond geometry as shown.

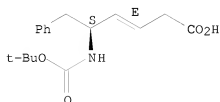


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

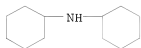
L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-,
[S-(E)]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI)
MF C17 H23 N O4 . C12 H23 N

CM 1

Absolute stereochemistry.
Double bond geometry as shown.

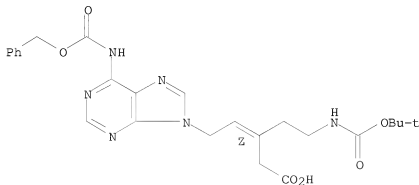


CM 2



L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Pentenoic acid, 3-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-5-[6-
[[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]-, (3Z)-
MF C25 H30 N6 O6

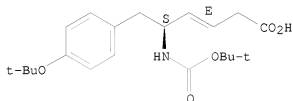
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-dimethylethoxy)phenyl]-, [S-(E)]- (9CI)
 MF C21 H31 N O5
 CI COM

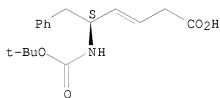
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-, (S)- (9CI)
 MF C17 H23 N O4

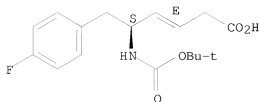
Absolute stereochemistry.
 Double bond geometry unknown.



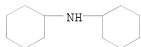
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(4-fluorophenyl)-, [S-(E)]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI)
 MF C17 H22 F N O4 . C12 H23 N
 CM 1

Absolute stereochemistry.
 Double bond geometry as shown.

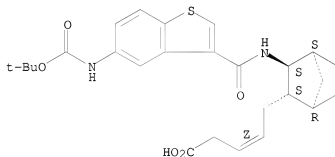


CM 2



L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[(1R,2S,3S,4S)-3-[[[5-[[[(1,1-dimethylethoxy)carbonyl]amino]benzo[b]thien-3-yl]carbonyl]amino]bicyclo[2.2.1]hept-2-yl]-, (3Z)-
 MF C26 H32 N2 O5 S

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.

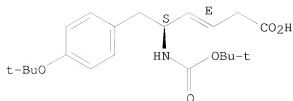


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

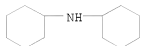
L22 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-dimethylethoxy)phenyl]-, [S-(E)]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI)
 MF C21 H31 N O5 . C12 H23 N

CM 1

Absolute stereochemistry.
 Double bond geometry as shown.



CM 2



ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
48.93	637.06

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-6.80

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 06:31:39 ON 07 APR 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

***** Welcome to STN International *****

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 12	Match STN Content and Features to Your Information Needs, Quickly and Conveniently
NEWS	3	JAN 25	Annual Reload of MEDLINE database
NEWS	4	FEB 16	STN Express Maintenance Release, Version 8.4.2, Is Now Available for Download
NEWS	5	FEB 16	Derwent World Patents Index (DWPI) Revises Indexing of Author Abstracts
NEWS	6	FEB 16	New FASTA Display Formats Added to USGENE and PCTGEN
NEWS	7	FEB 16	INPADOCDB and INPAFAMDB Enriched with New Content

and Features
 NEWS 8 FEB 16 INSPEC Adding Its Own IPC codes and Author's E-mail
 Addresses
 NEWS 9 APR 02 CAS Registry Number Crossover Limits Increased to
 500,000 in Key STN Databases
 NEWS 10 APR 02 PATDPAFULL: Application and priority number formats
 enhanced
 NEWS 11 APR 02 DWPI: New display format ALLSTR available
 NEWS 12 APR 02 New Thesaurus Added to Derwent Databases for Smooth
 Sailing through U.S. Patent Codes
 NEWS 13 APR 02 EMBASE Adds Unique Records from MEDLINE, Expanding
 Coverage back to 1948
 NEWS 14 APR 07 CA/CAPLUS CLASS Display Streamlined with Removal of
 Pre-IPC 8 Data Fields
 NEWS 15 APR 07 50,000 World Traditional Medicine (WTM) Patents Now
 Available in CAPLUS
 NEWS 16 APR 07 MEDLINE Coverage Is Extended Back to 1947
 NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
 AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.
 NEWS HOURS STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that
 specific topic.

All use of STN is subject to the provisions of the STN customer
 agreement. This agreement limits use to scientific research. Use
 for software development or design, implementation of commercial
 gateways, or use of CAS and STN data in the building of commercial
 products is prohibited and may result in loss of user privileges
 and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 08:45:40 ON 07 APR 2010

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 08:46:11 ON 07 APR 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
 SESSION RESUMED IN FILE 'HOME' AT 08:53:37 ON 07 APR 2010
 FILE 'HOME' ENTERED AT 08:53:37 ON 07 APR 2010

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
----------------------	------------	-------

	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.44	0.44

FILE 'REGISTRY' ENTERED AT 08:54:18 ON 07 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0
DICTIONARY FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e heptanoic acid, 7-phenyl-/cn

E1	1	HEPTANOIC ACID, 7-PHENOXY-, SILYL ESTER/CN
E2	1	HEPTANOIC ACID, 7-PHENOXY-, TRIMETHYLSILYL ESTER/CN
E3	2 -->	HEPTANOIC ACID, 7-PHENYL-/CN
E4	1	HEPTANOIC ACID, 7-PHENYL-, 1-ETHYL ESTER/CN
E5	1	HEPTANOIC ACID, 7-PHENYL-, PHENYL ESTER/CN
E6	1	HEPTANOIC ACID, 7-PIPERIDINO-/CN
E7	1	HEPTANOIC ACID, 7-PURIN-6-YLAMINO-/CN
E8	1	HEPTANOIC ACID, 7-SELENIINO-/CN
E9	1	HEPTANOIC ACID, 7-SULFANILAMIDO-/CN
E10	1	HEPTANOIC ACID, 7-SULFO-, 1-METHYL ESTER/CN
E11	1	HEPTANOIC ACID, 7-SULFO-, 1-METHYL ESTER, SODIUM SALT/CN
E12	1	HEPTANOIC ACID, 7-SULFO-, 1-METHYL ESTER, SODIUM SALT (1:1)/CN

=> e3

L1 2 "HEPTANOIC ACID, 7-PHENYL-"/CN

=> d l1

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2010 ACS on STN
RN 40228-90-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzeneheptanoic acid (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Heptanoic acid, 7-phenyl- (6CI, 7CI)
OTHER NAMES:
CN 7-Phenylheptanoic acid

MF C13 H18 O2
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS,
CSCHEM, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)

HO₂C-(CH₂)₆-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

97 REFERENCES IN FILE CA (1907 TO DATE)
98 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	8.58	9.02

FILE 'CAPLUS' ENTERED AT 08:55:21 ON 07 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 7 Apr 2010 VOL 152 ISS 15
FILE LAST UPDATED: 6 Apr 2010 (20100406/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2010

Caplus now includes complete International Patent Classification (IPC) reclassification data for the first quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

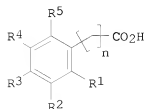
=> 11/thu
99 L1
1229755 THU/RL
L2 3 L1/THU
(L1 (L) THU/RL)

=> d 12 1-3 ti fbib abs

L2 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Phenylalkylcarboxylic acid delivery agents for biologically active compounds
 AN 2008:1128306 CAPLUS <<LOGINID:20100407>>
 DN 149:355552
 TI Phenylalkylcarboxylic acid delivery agents for biologically active compounds
 IN Pusztay, Stephen V.; Gacheidner, David
 PA Emisphere Technologies, Inc., USA
 SO PCT Int. Appl., 49pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2008112368	A2	20080918	WO 2008-US53429	20080208
	WO 2008112368	A3	20081120		
	W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
	RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
	CA 2676930	A1	20080918	US 2007-888927P	P 20070208
				CA 2008-2676930	20080208
				US 2007-888927P	P 20070208
				WO 2008-US53429	W 20080208
	EP 2114145	A2	20091111	EP 2008-782758	20080208
	R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR			
				US 2007-888927P	P 20070208
				WO 2008-US53429	W 20080208
	MX 2009008542	A	20091110	MX 2009-8542	20090807
				US 2007-888927P	P 20070208
				WO 2008-US53429	W 20080208
	CN 101616583	A	20091230	CN 2008-80004481	20090807
				US 2007-888927P	P 20070208
				WO 2008-US53429	W 20080208

OS MARPAT 149:355552
 GI



AB The present invention provides phenylalkylcarboxylic acid compds. of general formula I (wherein n is 1-12, and R1-R5 are independently H, C1-C6 alkyl, C2-C4 alkenyl, halo, C1-C4 alkoxy, hydroxy, C6-C14 aryloxy, or C1-C6 alkylhalo group) and compns. containing such compds. which facilitate the delivery of biol. active agents. Some of the phenylalkylcarboxylic acids are purchased and others are synthesized. Example compound 4-(4-methoxyphenyl)butanoic acid (II) was prepared by reacting anisole and succinic anhydride to give 4-(4-methoxyphenyl)-4-oxobutyric acid which was converted to II. Oral delivery of human zinc insulin (0.5 mg/kg) with II (200 mg/kg) as the delivery agent caused a 43.6 % reduction in blood glucose levels in rats.

L2 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2010 ACS on STN

TI Induction of histone acetylation and inhibition of growth by phenyl alkanolic acids and structurally related molecules

AN 2004:450167 CAPLUS <<LOGINID::20100407>>

DN 142:32394

TI Induction of histone acetylation and inhibition of growth by phenyl alkanolic acids and structurally related molecules

AU Lea, Michael A.; Shareef, Asif; Sura, Monali; desBordes, Charles

CS Department of Biochemistry and Molecular Biology, UMDNJ-New Jersey Medical School, Newark, NJ, 07103, USA

SO Cancer Chemotherapy and Pharmacology (2004), 54(1), 57-63

CODEN: CCPHDZ; ISSN: 0344-5704

PB Springer-Verlag

DT Journal

LA English

AB Purpose. A structure-activity study was undertaken to determine the influence of side chain length of Ph alkanolic acids and the degree of unsatn. of Ph alkenolic acids on the induction of histone acetylation and inhibition of cancer cell proliferation. Materials and methods. Studies on cell proliferation were performed with DS19 mouse erythroleukemic cells, PC-3 human prostate cancer cells and Caco-2 human colon cancer cells. Actions on histone deacetylase and the induction of histone acetylation were compared for 4-phenylbutyrate and structurally related mols. Results. Increasing inhibition of cell proliferation by Ph alkanolic acids together with a decrease in cells in S phase and an increase in apoptotic cells was observed with increased chain length between four and ten carbons. Introduction of double bonds into the side chain was associated with increased growth inhibition. In contrast, 4-phenylbutyrate was a more potent inhibitor of histone deacetylase and inducer of histone acetylation than the other Ph alkanolic acids examined. Conclusions. In comparison with the action of 4-phenylbutyrate, actions other than inhibition of histone deacetylase appear to be more important for growth inhibition by longer chain Ph alkanolic and Ph alkenolic acids.

OSC.G 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2010 ACS on STN

TI Skin permeation model of phenylalkylcarboxylic homologous acids and their enhancer effect on percutaneous penetration of 5-fluorouracil

AN 1996:491380 CAPLUS <<LOGINID::20100407>>

DN 125:204211

OREF 125:38056h,38057a

TI Skin permeation model of phenylalkylcarboxylic homologous acids and their enhancer effect on percutaneous penetration of 5-fluorouracil

AU Lopez, A.; Morant, M. J.; Guzman, D.; Borrás-Blasco, J.; Díez-Sales, O.; Herrera, M.

CS Departamento de Farmacia y Tecnologia Farmaceutica, Facultad de Farmacia,
 Universidad de Valencia, Avda. Vicente Andres Estelles s/n. 46100
 Burjassot, Valencia, Spain

SO International Journal of Pharmaceutics (1996), 139(1,2), 205-213
 CODEN: IJPHDE; ISSN: 0378-5173

PB Elsevier
 DT Journal
 LA English

AB This study was conducted primarily to establish the rat skin penetration
 model of acidic homologous series with a wide range of lipophilicity (from
 phenylpropionic acid to phenylcaprylic acid), and to compare it with other
 homologous series (alkylanilines) by means of adequate
 permeability-partition correlations, in order to find out if there could
 be a common model of penetration for all the compds. The influence of pH
 on acid penetration through the skin was also analyzed. Standard in vitro
 skin permeation methods using rat skin were used to determine the permeability
 coeffs. of phenylalkylcarboxylic acids in the conditions established.
 Membrane/water partition coeffs. were also assessed, and the correlations
 between permeability and partition values were established. A linear
 relationship between the logarithms of permeabilities of penetrants and
 the corresponding membrane/water partition coeffs. was found. The
 apparent discordance between this type of correlation and the
 probabilistic (i.e. parabolic) model previously established with other
 homologous series (alkylanilines) is attributed to a self-enhancing effect
 on penetration in the case of the more lipophilic compds. of the series.
 In fact, when 5-FU was used as a polar model permeant, pretreatment of the
 membrane with phenylenanthic acid gave it an enhancer ratio of 4.5, thus
 confirming its enhancer effect.

OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

=> logoff hold
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
23.61	32.63
SINCE FILE	TOTAL
ENTRY	SESSION
-2.55	-2.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
 CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 09:09:34 ON 07 APR 2010
 Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

***** RECONNECTED TO STN INTERNATIONAL *****
 SESSION RESUMED IN FILE 'CAPLUS' AT 09:49:45 ON 07 APR 2010
 FILE 'CAPLUS' ENTERED AT 09:49:45 ON 07 APR 2010
 COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
23.61	32.63

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-2.55	-2.55

```
=> file reg
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          24.11      33.13
```

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-2.55	-2.55

FILE 'REGISTRY' ENTERED AT 09:50:08 ON 07 APR 2010
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0
 DICTIONARY FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> FIL STNGUIDE
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          0.49      33.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                                ENTRY      SESSION
CA SUBSCRIBER PRICE                                0.00      -2.55
```

FILE 'STNGUIDE' ENTERED AT 09:50:25 ON 07 APR 2010
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
 COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
 LAST RELOADED: Apr 2, 2010 (20100402/UP).

```
=> DIS SAVED
NAME      CREATED      NOTES/TITLE
-----
ALKCARBFNDS/A  24 JUL 2006  1991 ANSWERS IN FILE REGISTRY
ANTBACCORE/A   TEMP        325 ANSWERS IN FILE REGISTRY
MASTERSET/A    TEMP        24701 ANSWERS IN FILE REGISTRY
```

MSTRUNSATS/A	TEMP	222 ANSWERS IN FILE REGISTRY
PLYETHRAMINS/A	13 JUL 2007	299 ANSWERS IN FILE REGISTRY
PPARAWCMPDS/A	29 OCT 2009	2046 ANSWERS IN FILE REGISTRY
RAWRXNS/A	22 SEP 2008	36 ANSWERS IN FILE CASREACT
REFNDFNDS/A	24 JUL 2006	1255 ANSWERS IN FILE REGISTRY
TBUTCARBFNDS/A	24 JUL 2006	736 ANSWERS IN FILE REGISTRY
THIAFNDS/A	06 FEB 2007	113 ANSWERS IN FILE REGISTRY
TWOAMINOPOLY/Q	16 APR 2001	UPLOADED STRUCTURE
Y2BONDMSTR/A	TEMP	1810 ANSWERS IN FILE REGISTRY

=> DIS SAVED/S
NO SAVED SDI REQUESTS

=> FIL REGISTRY		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.07	33.69
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		
	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.55

FILE 'REGISTRY' ENTERED AT 09:51:15 ON 07 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0
DICTIONARY FILE UPDATES: 5 APR 2010 HIGHEST RN 1217056-90-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

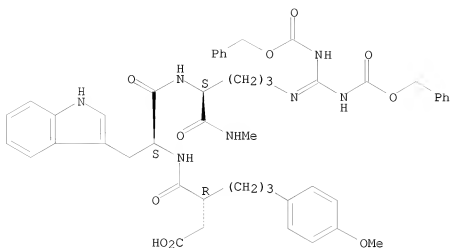
<http://www.cas.org/support/stngen/stndoc/properties.html>

=> ACT Y2BONDMSTR/A
L3 STR
L4 1810 SEA FILE=REGISTRY SSS FUL L3

=> d scan

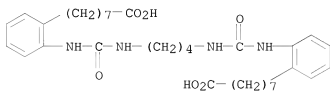
L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN L-Ornithinamide, N-[(2R)-2-(carboxymethyl)-5-(4-methoxyphenyl)-1-oxopentyl]-L-tryptophyl-N5-[bis[[[phenylmethoxy]carbonyl]amino]methylene]-N-methyl-
MF C48 H55 N7 O10

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C34 H50 N4 O6

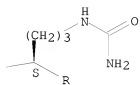
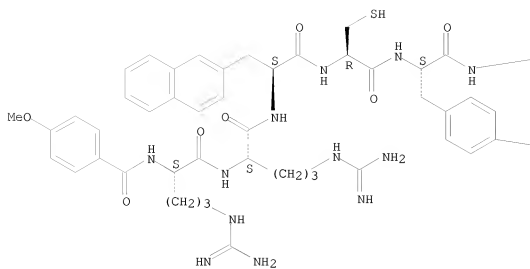


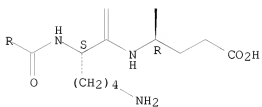
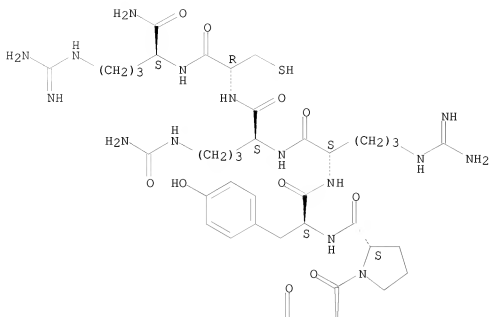
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 SQL 14
 MF C97 H144 N32 O22 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

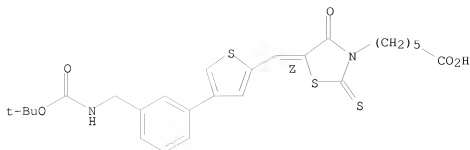




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Thiazolidinehexanoic acid, 5-[[[4-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]phenyl]-2-thienyl]methylene]-4-oxo-2-thioxo-, (5Z)-
 MF C26 H30 N2 O5 S3

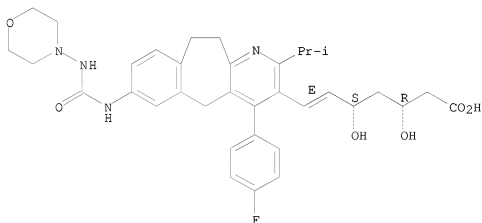
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 6-Heptenoic acid, 7-[4-(4-fluorophenyl)-10,11-dihydro-2-(1-methylethyl)-7-
 [[(4-morpholinylamino) carbonyl] amino]-5H-benzo[4,5]cyclohepta[1,2-
 b]pyridin-3-yl]-3,5-dihydroxy-, (3R,5S,6E)-
 MF C35 H41 F N4 O6

Absolute stereochemistry.
 Double bond geometry as shown.

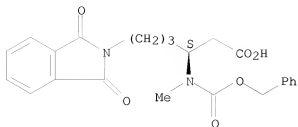


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2H-isoindole-2-hexanoic acid, 1,3-dihydro-β-
 [methyl[(phenylmethoxy) carbonyl] amino]-1,3-dioxo-, compd. with
 2-methyl-2-propanamine (1:1), (βS)-
 MF C23 H24 N2 O6 . C4 H11 N

CM 1

Absolute stereochemistry.

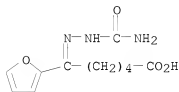


CM 2



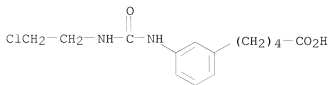
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 2-Furanhexanoic acid, *s*-[2-(aminocarbonyl)hydrazinyldene]-
 MF C11 H15 N3 O4



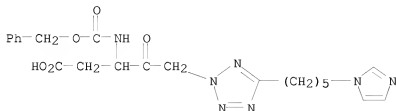
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Benzenepentanoic acid, 3-[[[(2-chloroethyl)amino]carbonyl]amino]-
 MF C14 H19 Cl N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2H-Tetrazole-2-pentanoic acid, 5-[5-(1H-imidazol-1-yl)pentyl]-γ-oxo-
β-[(phenylmethoxy)carbonyl]amino]-
MF C22 H27 N7 O5
CI COM

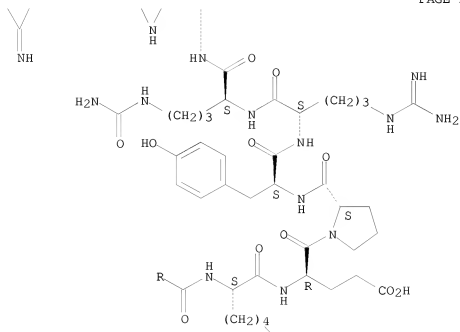
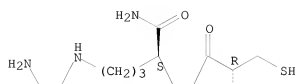
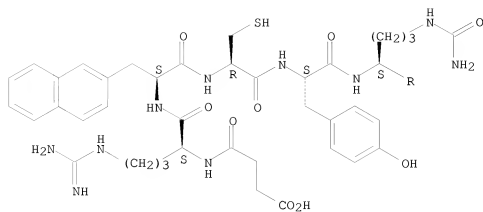


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN L-Argininamide, N2-(3-carboxy-1-oxopropyl)-L-arginyl-3-(2-naphthalenyl)-L-
alanyl-L-cysteinyl-L-tyrosyl-N5-(aminocarbonyl)-L-ornithyl-L-lysyl-D-
α-glutamyl-L-prolyl-L-tyrosyl-L-arginyl-N5-(aminocarbonyl)-L-
ornithyl-L-cysteinyl-
SQL 13
MF C87 H130 N28 O22 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

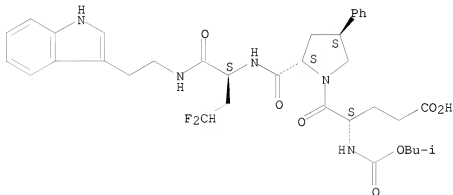




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 1810 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN Butanamide, N-[(2-methylpropoxy)carbonyl]-L- α -glutamyl-(4S)-4-phenyl-
 L-prolyl-2-amino-4,4-difluoro-N-[2-(1H-indol-3-yl)ethyl]-, (2S)- (9CI)
 MF C35 H43 F2 N5 O7

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
 files\10025947\10025947 unsatsy2bond.str

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 O,N

G2 O,S,N,[@1-@2]

Structure attributes must be viewed using STN Express query preparation.

=> search l5 sss sam

SAMPLE SEARCH INITIATED 09:53:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1204 TO ITERATE

100.0% PROCESSED 1204 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 21999 TO 26161

PROJECTED ANSWERS: 2 TO 124

L6 2 SEA SSS SAM L5

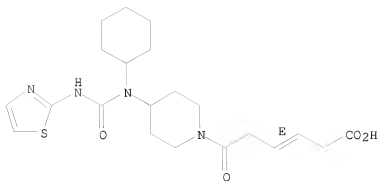
=> d scan

L6 2 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 3-Hexenoic acid, 6-[4-[cyclohexyl[(2-thiazolylamino)carbonyl]amino]-1-piperidinyl]-6-oxo-, (3E)-

MF C21 H30 N4 O4 S

Double bond geometry as shown.

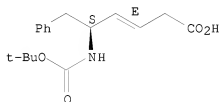


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 2 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-,
 (3E,5S)-
 MF C17 H23 N O4
 CI COM

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search 15 sss full
 FULL SEARCH INITIATED 09:54:33 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 23846 TO ITERATE

100.0% PROCESSED 23846 ITERATIONS
 SEARCH TIME: 00.00.03

39 ANSWERS

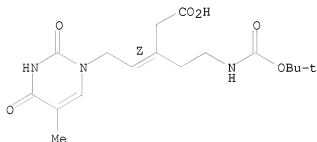
L7 39 SEA SSS FUL L5

=> d scan

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-3-

[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (3Z)-
MF C17 H25 N3 O6

Double bond geometry as shown.

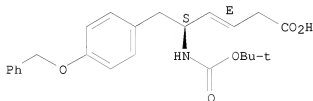


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):39

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(phenylmethoxy)phenyl]-, [S-(E)]- (9CI)
MF C24 H29 N O5

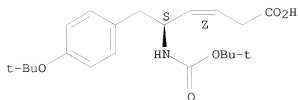
Absolute stereochemistry.
Double bond geometry as shown.



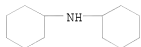
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-dimethylethoxy)phenyl]-, [S-(Z)]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI)
MF C21 H31 N O5 . C12 H23 N
CM 1

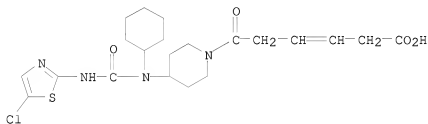
Absolute stereochemistry.
Double bond geometry as shown.



CM 2



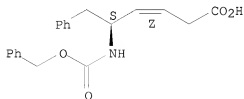
L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-[4-[[[(5-chloro-2-thiazolyl)amino]carbonyl]cyclohexylamino]-1-piperidinyl]-6-oxo-
 MF C21 H29 Cl N4 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[[(phenylmethoxy)carbonyl]amino]-, (3Z,5S)-
 MF C20 H21 N O4

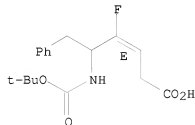
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
, (E)- (9CI)
MF C17 H22 F N O4

Double bond geometry as shown.

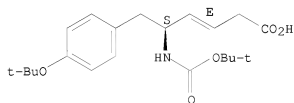


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

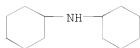
L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-dimethylethoxy)phenyl]-, [S-(E)]-, compd. with N-cyclohexylcyclohexanamine
(1:1) (9CI)
MF C21 H31 N O5 . C12 H23 N

CM 1

Absolute stereochemistry.
Double bond geometry as shown.



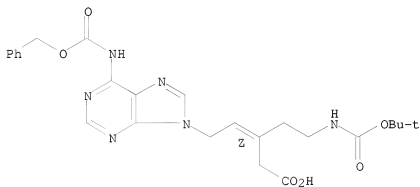
CM 2



L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 3-Pentenoic acid, 3-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-5-[6-
 MF [[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]-, (3Z)-
 C25 H30 N6 O6

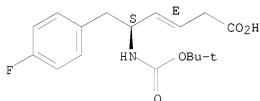
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(4-
 MF fluorophenyl)-, [S-(E)]- (9CI)
 CI C17 H22 F N O4
 COM

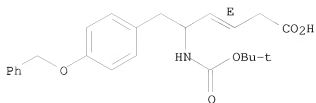
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-
 MF (phenylmethoxy)phenyl]-, (3E)-
 C24 H29 N O5

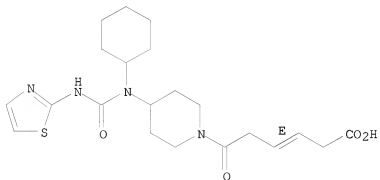
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-[4-(cyclohexyl[(2-thiazolylamino)carbonyl]amino)-1-piperidinyl]-6-oxo-, (3E)-
 MF C21 H30 N4 O4 S

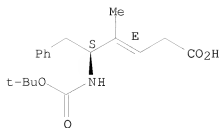
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-6-phenyl-1,1-dimethylethoxy]-, [S-(E)]- (9CI)
 MF C18 H25 N O4

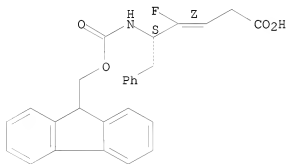
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, (3Z,5S)-
 MF C27 H24 F N O4

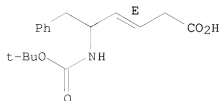
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-, (E)-
 (9CI)
 MF C17 H23 N O4

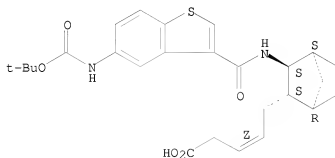
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[(1R,2S,3S,4S)-3-[[[5-[(1,1-dimethylethoxy)carbonyl]amino]benzo[b]thien-3-yl]carbonyl]amino]bicyclo[2.2.1]hept-2-yl]-, (3Z)-
 MF C26 H32 N2 O5 S

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.

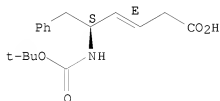


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

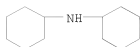
L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-, [S-(E)]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI)
 MF C17 H23 N O4 . C12 H23 N

CM 1

Absolute stereochemistry.
 Double bond geometry as shown.

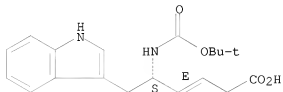


CM 2



L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(1H-indol-3-yl)-
 , [S-(E)]- (9CI)
 MF C19 H24 N2 O4

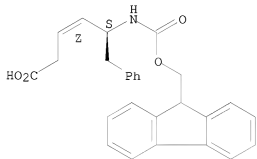
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-6-phenyl-,
 (3Z,5S)- (9CI)
 MF C27 H25 N O4

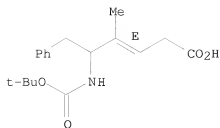
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-6-phenyl-,
 , (E)- (9CI)
 MF C18 H25 N O4

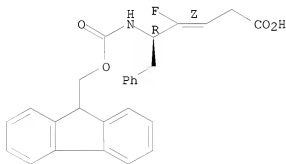
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[9H-fluoren-9-ylmethoxy]carbonyl]amino]-4-fluoro-6-phenyl-, [R-(Z)]-, (9CI)
 MF C27 H24 F N O4

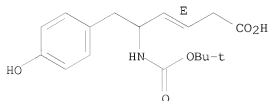
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[1,1-dimethylethoxy]carbonyl]amino]-6-(4-hydroxyphenyl)-, (E)- (9CI)
 MF C17 H23 N O5

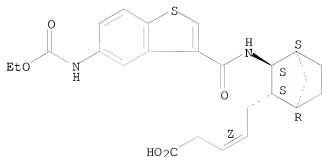
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Pentenoic acid, 5-[(1R,2S,3S,4S)-3-[[[5-
 [(ethoxycarbonyl)amino]benzo[b]thien-3-
 yl]carbonyl]amino]bicyclo[2.2.1]hept-2-yl]-, (3Z)-
 MF C24 H28 N2 O5 S

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.

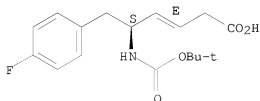


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

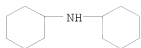
L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-(4-
 fluorophenyl)-, [S-(E)]-, compd. with N-cyclohexylcyclohexanamine (1:1)
 (9CI)
 MF C17 H22 F N O4 . C12 H23 N

CM 1

Absolute stereochemistry.
 Double bond geometry as shown.

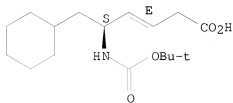


CM 2



L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-cyclohexyl-5-[[[(1,1-dimethylethoxy)carbonyl]amino]-,
 [S-(E)]- (9CI)
 MF C17 H29 N O4

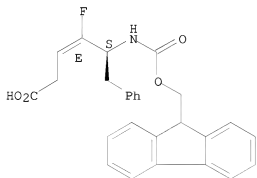
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-
 phenyl-, (3E,5S)-
 MF C27 H24 F N O4

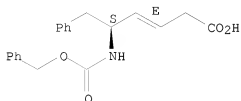
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[[(phenylmethoxy)carbonyl]amino]-, [S-(E)]-
 (9CI)
 MF C20 H21 N O4

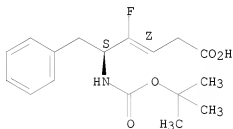
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
, [S-(Z)]- (9CI)
MF C17 H22 F N O4

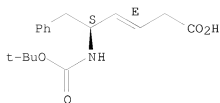
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-,
(3E,5S)-
MF C17 H23 N O4
CI COM

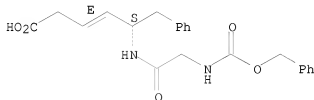
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 6-phenyl-5-[[2-
 [[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, (3E,5S)-
 MF C22 H24 N2 O5

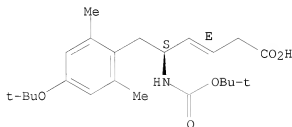
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[[4-(1,1-
 dimethylethoxy)-2,6-dimethylphenyl]-, [S-(E)]- (9CI)
 MF C23 H35 N O5

Absolute stereochemistry.
 Double bond geometry as shown.

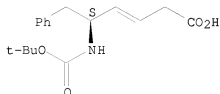


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-, (S)-
(9CI)
MF C17 H23 N O4

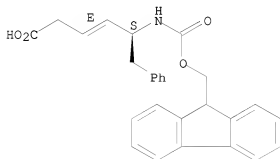
Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-6-phenyl-,
(3E,5S)-
MF C27 H25 N O4

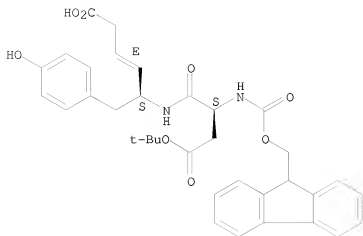
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Hexenoic acid, 5-[[[(2S)-4-(1,1-dimethylethoxy)-2-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1,4-dioxobutyl]amino]-6-(4-hydroxyphenyl)-,
(3E,5S)-
MF C35 H38 N2 O8

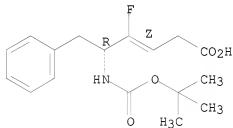
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
 , [R-(Z)]- (9CI)
 MF C17 H22 F N O4

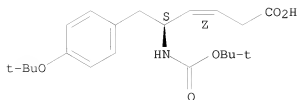
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-
 dimethylethoxy)phenyl]-, [S-(Z)]- (9CI)
 MF C21 H31 N O5
 CI COM

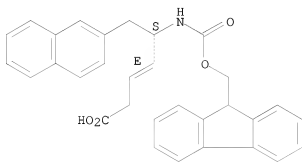
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[9H-fluoren-9-ylmethoxy]carbonyl]amino]-6-(2-naphthalenyl)-, (3E,5S)-
 MF C31 H27 N O4

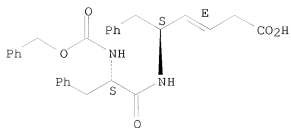
Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[1-oxo-3-phenyl-2-[[[phenylmethoxy]carbonyl]amino]propyl]amino]-6-phenyl]-, [S-[R*,R*-(E)]]-(9CI)
 MF C29 H30 N2 O5

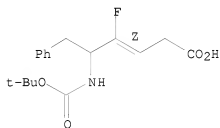
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-
 , (Z)- (9CI)
 MF C17 H22 F N O4

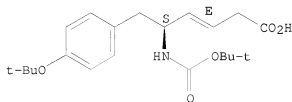
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 39 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Hexenoic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-[4-(1,1-
 dimethylethoxy)phenyl]-, [S-(E)]- (9CI)
 MF C21 H31 N O5
 CI COM

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e 3-hexenoic acid, 5-amino-4-phenyl-/cn
E1 1 3-HEXENOIC ACID, 5-AMINO-4-FLUORO-6-PHENYL-, (3Z,5S)-, 2,2,2-TRIFLUOROACETATE (1:1)/CN
E2 1 3-HEXENOIC ACID, 5-AMINO-4-FLUORO-6-PHENYL-, (3Z,5S)-, TRIFLUOROACETATE/CN
E3 0 --> 3-HEXENOIC ACID, 5-AMINO-4-PHENYL-/CN
E4 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5S)-/CN
E5 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5S)-, 2,2,2-TRIFLUOROACETATE (1:1)/CN
E6 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5S)-, TRIFLUOROACETATE/CN
E7 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3Z,5S)-, 2,2,2-TRIFLUOROACETATE (1:1)/CN
E8 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (S-(Z))-/CN
E9 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (S-(Z))-, TRIFLUOROACETATE/CN
E10 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, HYDROCHLORIDE (1:1), (3E,5S)-/CN
E11 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, HYDROCHLORIDE, (S-(E))-/CN
E12 1 3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, METHYL ESTER, (S-(E))-/CN

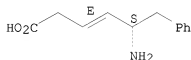
=> e4

L8 1 "3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5S)-"/CN

=> d 18

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN
RN 521064-20-0 REGISTRY
ED Entered STN: 27 May 2003
CN 3-Hexenoic acid, 5-amino-6-phenyl-, (3E,5S)- (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H15 N O2
CI COM
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST	ENTRY 204.04	SESSION 237.73
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.55

FILE 'CAPLUS' ENTERED AT 09:57:46 ON 07 APR 2010
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 7 Apr 2010 VOL 152 ISS 15
 FILE LAST UPDATED: 6 Apr 2010 (20100406/ED)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2010
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2010

Caplus now includes complete International Patent Classification (IPC) reclassification data for the first quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l8

L9 1 L8

=> d l9 ti fbib abs

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN
 TI Design and synthesis of amide isosteres of Phe-Gly: potential peptidomimetic ligands for the intestinal oligopeptide transporter PepT1
 AN 2002:692505 CAPLUS <LOGINID:20100407>
 DN 138:354217
 TI Design and synthesis of amide isosteres of Phe-Gly: potential peptidomimetic ligands for the intestinal oligopeptide transporter PepT1
 AU Vabeno, Jon; Brisander, Magnus; Chen, Weiqing; Borchardt, Ronald T.; Luthman, Kristina
 CS Department of Medicinal Chemistry, University of Tromso, Tromso, N-9037, Norway
 SO Peptides: The Wave of the Future, Proceedings of the Second International and the Seventeenth American Peptide Symposium, San Diego, CA, United States, June 9-14, 2001 (2001), 610-611. Editor(s): Lebl, Michal; Houghten, Richard A. Publisher: American Peptide Society, San Diego, Calif.
 CODEN: 69DBAL; ISBN: 0-9715560-0-8
 DT Conference

LA English

AB A symposium report. The transport of di- and tripeptides across the intestinal epithelium is an active process mediated by the oligopeptide transporter PepT1. Synthetic Phe-Gly peptidomimetics, where amide bond was replaced by isosteric moieties, were used in preliminary transport studies on Caco-2 cells.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
4.10	241.83

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.85	-3.40

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 09:58:45 ON 07 APR 2010